**Unified Manifold-Based Approach to Modeling Turbulent Combustion in LES**

In practical combustion systems, rapid mixing is required to achieve shorter residence times. This is where the importance of turbulent combustion comes into play. Nonlinear, multi-scale interactions of turbulence, molecular transport, and combustion chemistry characterize turbulent combustion. Direct Numerical Simulation (DNS) resolves all continuum scales, but the computational cost is extremely expensive and unlikely to be adaptable for predicting practical combustion systems. Instead of resolving all scales, Large Eddy Simulation (LES) only resolves large scales and models small scales, which significantly reduces the computational cost compared to DNS. In particular, because LES resolves large-scale mixing processes important in turbulent combustion, LES yields better predictions of turbulent combustion than Reynolds-Averaged Navier-Stokes (RANS), which models all scales [1]. However, modeling turbulent combustion in LES requires closure models for unclosed terms, which can capture turbulence-chemistry interactions. Thus, the focus of my research is to address the challenges in LES modeling of turbulent combustion.

The effects of turbulence on flame structure and combustion heat release have been extensively studied and applied to modeling filtered molecular transport and chemical source terms [2]. In contrast, the influence of combustion heat release on small-scale turbulence has been overlooked. Models for subfilter stresses and scalar fluxes typically rely on turbulence models originally developed for non-reacting flows. This implicitly assumes that combustion heat release does not affect small-scale turbulence. However, combustion heat release induces flow dilatation driven by thermal expansion in the flame, and pressure-dilatation work appears as a small-scale source term for turbulent kinetic energy (TKE) [3]. In the context of scaling arguments, the importance of combustion heat release is augmented when its time and length scales are faster and smaller compared to those of turbulence [4].

When combustion heat release strongly affects turbulence, thermal expansion in the flame accelerates the flow velocity in the flame normal direction. This results in counter-Boussinesq and counter-gradient transport for subfilter stresses and scalar fluxes, respectively [5]. Recently, an algebraic heat release model was developed to consider the effects of combustion heat release on the Reynolds stresses and scalar fluxes in a RANS context [6], which was also extended to the subfilter stresses and scalar fluxes in LES [7]. This approach linearly combines two models in limiting states (i.e., infinite and zero Karlovitz number, $Ka$, defined as the ratio of flame and Kolmogorov time scales), and better predicts the flame-normal component of subfilter stresses and scalar fluxes in turbulent premixed combustion. However, it has limitations in capturing effects of nonlinear turbulence-heat release interaction and finite flame thickness, and it is not applicable to non-premixed and multi-modal combustion.

In my research, a more complete model will be developed. Velocity and scalars are conditioned on a flame structure variable (e.g., progress variable in premixed combustion, mixture fraction in non-premixed combustion, or both in multi-modal combustion). As turbulence is locally coupled with flame motion, both turbulence and flame motion affect unconditional statistics. Conditioning on a flame structure variable separates the effects of flame motion from the direct effects of combustion heat release [8]. Therefore, flame-conditioned statistics are more representative of turbulence than unconditional statistics. In addition, given that combustion heat release depends on flame structure, conditioning makes it more tractable to develop closure models for transport equations for flame-conditioned variables with an emphasis on combustion heat release.

This new approach generalizes the model with flame-conditioned scalars referred to as Conditional Moment Closure (CMC) [9]. In CMC, transport equations are solved for flame-conditioned scalars. As subfilter variations in the flame structure variable are captured in CMC, first-order closure is capable of capturing the filtered chemical source term. In this conventional approach, the conditionally filtered velocity is commonly modeled by simply using the unconditionally filtered value in the CMC equation. However, this approximation neglects the influence of combustion heat release on turbulence as conditionally filtered velocity has variation in the flame structure variable. In considering turbulence and combustion together by simultaneously solving conditionally filtered transport equations for both velocity and scalars, this new way of modeling serves as the basis for a unified manifold-based approach.

In LES for turbulent premixed combustion, density-weighted conditional filtering for a quantity $\phi$ is defined as

$$\tilde{\Phi}_{\lambda} = \frac{\int \rho(x_j',t)\phi(x_j',t)\delta[\lambda - \Lambda(x_j',t)]G(x_j' - x_j;\Delta)dx_j'}{\int \rho(x_j',t)\delta[\lambda - \Lambda(x_j',t)]G(x_j' - x_j;\Delta)dx_j'} \quad (1)$$

where $\rho$ is the density, $\lambda$ is the phase-space variable for a progress variable $\Lambda$, $\delta$ is Dirac delta function, $G$ is the filter kernel, $\Delta$ is the filter width, $\tilde{}$ indicates density-weighted filtered quantity, and subscript $\lambda$ indicates that the quantity is conditionally filtered on $\lambda$. Conditionally filtered transport equations for velocity $u_i$ and species mass fraction $Y_k$ are derived following the joint PDF method [9]:

$$\begin{aligned}\frac{\partial \tilde{u}_{i\lambda}}{\partial t} + \tilde{u}_{j\lambda}\frac{\partial \tilde{u}_{i\lambda}}{\partial x_j} = &-\frac{1}{\bar{\rho}\tilde{P}}\left[\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{P}\widetilde{u_i u_j}_{\lambda} - \bar{\rho}\tilde{P}\tilde{u}_{i\lambda}\tilde{u}_{j\lambda}\right) + \frac{\partial^2}{\partial x_j \partial \lambda}\left(\bar{\rho}\tilde{P}\left\{u_i D_{\Lambda}\frac{\partial \Lambda}{\partial x_j}\right\}_{\lambda}\right) - \tilde{u}_{i\lambda}\frac{\partial^2}{\partial x_j \partial \lambda}\left(\bar{\rho}\tilde{P}\left\{D_{\Lambda}\frac{\partial \Lambda}{\partial x_j}\right\}_{\lambda}\right)\right] - \frac{1}{\bar{\rho}_{\lambda}}\overline{\frac{\partial p}{\partial x_i}}_{\lambda} \\ &+ \frac{1}{\bar{\rho}_{\lambda}}\overline{\frac{\partial \tau_{ij}}{\partial x_i}}_{\lambda} - \frac{1}{\bar{\rho}_{\lambda}}\bar{\dot{m}}_{\Lambda\lambda}\frac{\partial \tilde{u}_{i\lambda}}{\partial \lambda} \\ &- \frac{1}{\bar{\rho}\tilde{P}}\left[\frac{\partial}{\partial \lambda}\left(\overline{u_i \dot{m}_{\Lambda}}_{\lambda}\tilde{P} - \tilde{u}_{i\lambda}\bar{\dot{m}}_{\Lambda\lambda}\tilde{P}\right) - \frac{\partial}{\partial \lambda}\left(\bar{\rho}\tilde{P}\left\{D_{\Lambda}\frac{\partial u_i}{\partial x_j}\frac{\partial \Lambda}{\partial x_j}\right\}_{\lambda}\right) + \frac{1}{2}\frac{\partial^2}{\partial \lambda^2}\left(\bar{\rho}\tilde{P}\widetilde{u_i \chi_{\Lambda}}_{\lambda}\right) - \frac{1}{2}\tilde{u}_{i\lambda}\frac{\partial^2}{\partial \lambda^2}\left(\bar{\rho}\tilde{P}\tilde{\chi}_{\Lambda\lambda}\right)\right]\end{aligned} \quad (2)$$

$$\begin{aligned}\frac{\partial \tilde{Y}_{k\lambda}}{\partial t} + \tilde{u}_{j\lambda}\frac{\partial \tilde{Y}_{k\lambda}}{\partial x_j} = &-\frac{1}{\bar{\rho}\tilde{P}}\left[\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{P}\widetilde{u_i Y_k}_{\lambda} - \bar{\rho}\tilde{P}\tilde{u}_{i\lambda}\tilde{Y}_{k\lambda}\right) + \frac{\partial^2}{\partial x_j \partial \lambda}\left(\bar{\rho}\tilde{P}\left\{Y_k D_{\Lambda}\frac{\partial \Lambda}{\partial x_j}\right\}_{\lambda}\right) - \tilde{Y}_{k\lambda}\frac{\partial^2}{\partial x_j \partial \lambda}\left(\bar{\rho}\tilde{P}\left\{D_{\Lambda}\frac{\partial \Lambda}{\partial x_j}\right\}_{\lambda}\right)\right] + \frac{1}{\bar{\rho}_{\lambda}}\bar{\dot{m}}_{k\lambda} \\ &+ \frac{1}{\bar{\rho}\tilde{P}}\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{P}\left\{D_k\frac{\partial Y_k}{\partial x_j}\right\}_{\lambda}\right) - \frac{1}{\bar{\rho}_{\lambda}}\bar{\dot{m}}_{\Lambda\lambda}\frac{\partial \tilde{Y}_{k\lambda}}{\partial \lambda} \\ &- \frac{1}{\bar{\rho}\tilde{P}}\left[\frac{\partial}{\partial \lambda}\left(\overline{Y_k \dot{m}_{\Lambda}}_{\lambda}\tilde{P} - \tilde{Y}_{k\lambda}\bar{\dot{m}}_{\Lambda\lambda}\tilde{P}\right) - \frac{\partial}{\partial \lambda}\left(\bar{\rho}\tilde{P}\left\{D_{\Lambda}\frac{\partial Y_k}{\partial x_j}\frac{\partial \Lambda}{\partial x_j}\right\}_{\lambda} + \bar{\rho}\tilde{P}\left\{D_k\frac{\partial Y_k}{\partial x_j}\frac{\partial \Lambda}{\partial x_j}\right\}_{\lambda}\right) + \frac{1}{2}\frac{\partial^2}{\partial \lambda^2}\left(\bar{\rho}\tilde{P}\widetilde{Y_k \chi_{\Lambda}}_{\lambda}\right) \right. \\ &\left. - \frac{1}{2}\tilde{Y}_{k\lambda}\frac{\partial^2}{\partial \lambda^2}\left(\bar{\rho}\tilde{P}\tilde{\chi}_{\Lambda\lambda}\right)\right]\end{aligned} \quad (3)$$

where $p$ is the hydrodynamic pressure, $\tau_{ij}$ is the viscous stress tensor, $D_{\Lambda}$ is the progress variable diffusivity, $\dot{m}_{\Lambda}$ is the progress variable source term, $\chi_{\Lambda}$ is the progress variable dissipation rate, $\tilde{P}$ is the density-weighted subfilter PDF of $\lambda$, $\bar{}$ indicates filtered quantity, and { } corresponds to $\tilde{}$. Convolution of conditionally filtered quantity and $\tilde{P}$ gives the corresponding filtered quantity.

Both conditionally filtered transport equations for velocity and species mass fraction are solved. Although conditional filtering results in high-dimensional equations with many unclosed terms, the development of closure models is expected to be more intuitive. Once conditioning on flame structure variable removes the effects of flame motion, closure models developed for unconditional terms could potentially be applied to analogous conditional terms (e.g., conditional subfilter stresses). In addition, the effects of combustion heat release are more simply introduced into modeling unclosed terms as turbulence is coupled with flame structure, and combustion heat release varies in flame structure.

By using the available DNS databases of turbulent hydrogen/air spatially-evolving planar jet flame in premixed and non-premixed configurations [6, 7, 8], budgets of Eq. 2 and 3 will be analyzed to determine dominant terms. Closure models will then be developed for unclosed terms, and both *a priori* and *a posteriori* validations will be performed by treating DNS data as an exact solution. As a final goal, the newly developed model will be tested against experimental data from a Cambridge Stratified Swirl Burner [10], where the detailed velocity measurement database is available for both premixed and stratified combustion, and turbulence is expected to be significantly affected by the effects of combustion heat release.

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