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Dynamic adaptive combustion modeling of spray flames based on chemical explosive mode analysis

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ABSTRACT

A dynamic adaptive combustion modeling framework based on chemical explosive mode analysis (CEMA) is proposed to account for different flame features such as local auto-ignition, premixed and non-premixed flamelets in diesel spray flames. The proposed modeling strategy is achieved by assigning zone-dependent combustion models on-the-fly to different flame zones segmented using a CEMA-based approach. An approximate CEMA formulation is developed to approximate the eigenvalue of the chemical explosive mode with high computational efficiency in three-dimensional (3-D) turbulent flame simulations. The utility of the CEMA-based criterion for dynamic flame segmentation is first demonstrated using CEMA-based adaptive chemistry by applying different reduced chemistry to different flame zones. The capability of the dynamic adaptive combustion modeling strategy is then demonstrated in large eddy simulations (LES) of turbulent lifted *n*-dodecane spray flames. Specifically, inert mixing is used for chemically inactive zones, and the well-mixed combustion model with finite rate chemistry is applied in the pre-ignition zone to capture the two-stage ignition as well as premixed reaction fronts. Adaptive mesh refinement (AMR) is further adopted near the premixed reaction fronts to capture the local flame structure and flame propagation speed. For the post-ignition zone, a recently developed tabulated flamelet model (TFM) is applied and compared with the flamelet progress variable (FPV) method. It is shown that CEMA-based adaptive chemistry induces small errors to the statistically-averaged flame structures, as CEMA is an effective and robust approach for on-the-fly flame segmentation. It is further seen that the CEMA-based adaptive modeling strategy more accurately predicts the ignition delay time and flame lift-off length compared with the low-cost flamelet models such as TFM and FPV, while the computational cost is substantially lower compared with the well-mixed combustion model using finite rate chemistry.

1. Introduction

Predictive simulations are important to improve the designs of advanced combustion engines. Among the different approaches for computational fluid dynamics (CFD) of turbulent combustion, direct numerical simulations (DNS) resolve all the temporal and spatial scales in turbulence and do not rely on turbulence and combustion models. However, DNS remain prohibitive for full-scale engine simulations due to the high computational cost. Instead, Reynolds-averaged Navier-Stokes (RANS) simulations with significantly lower computational cost have been widely adopted to assist engine design and optimization. Recently, due to the rapid increase in computer power, large eddy simulations (LES) have started to draw more attention in the engine combustion simulation community [1].

Both RANS and LES require turbulence and combustion modeling for closure of the averaged or filtered equations. Many turbulent combustion models have been developed in the literature [2], such as the well-mixed model [3,4], eddy dissipation concept (EDC) [5], and transported probability density function (PDF) method [6–8]. These methods typically involve finite rate chemistry and the computational cost can be high when using detailed chemical kinetics. The flamelet-type models assume a very-low-dimensional manifold in the composition space such that the solution can be indexed by one or a few variables for reduced computational cost. There are many variations of the flamelet

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model, such as the steady flamelet model [9], flamelet progress variable (FPV) model [10,11], flamelet generated manifold (FGM) [12], flame prolongation of intrinsic low-dimensional manifolds (FPI) [13], representative interactive flamelet (RIF) model [14], and the recently-developed tabulated flamelet model (TFM) [15,16]. The flamelet models nevertheless may fail where the very low-dimensional manifold assumption is not applicable, e.g. when the low-dimensional flame structures are destroyed by strong turbulence.

As another limitation, many turbulent combustion models and their coupled mixing models, such as the flamelet models, are specifically formulated and/or calibrated for either premixed or non-premixed flames, while in transient ignition process of the partially premixed diesel flames, non-premixed and premixed flame features can exist simultaneously. Therefore, it remains a challenge to accurately and efficiently model lifted diesel spray flames. Hybrid combustion models could provide a viable solution of this issue by applying different models in different flame zones, and several hybrid models have been developed for diesel combustion [17,18]. However, the model assignment and/or flame zone identification in such hybrid models are largely based on empirical or semi-empirical criteria.

In the present study, a high-fidelity dynamic adaptive combustion modeling framework is developed for non-premixed, premixed and partially premixed flames based on rigorous flame segmentation using the chemical explosive mode analysis (CEMA) [19–21], with appropriate models assigned on-the-fly to different flame zones for accurate and efficient simulations.

2. Methodology

2.1. Flame segmentation based on CEMA

Chemical explosive mode analysis (CEMA) [19–21] is a computational flame diagnostic based on eigen-analysis of the Jacobian of the local chemical source term in the governing equations of a reacting flow, which can be described by the following spatially discretized equations

$$\frac{D\boldsymbol{\omega}(\boldsymbol{y})}{Dt} = \mathbf{J}\cdot\frac{D\boldsymbol{y}}{Dt} = \mathbf{J}\cdot(\boldsymbol{\omega}+\boldsymbol{s}), \qquad \mathbf{J} = \frac{\partial\boldsymbol{\omega}}{\partial\boldsymbol{y}} \tag{1}$$

where $\boldsymbol{y}$ is the vector of local reacting variables, including temperature and species concentrations, $\boldsymbol{\omega}$ is the chemical source term, and $\boldsymbol{s}$ is the non-chemical source term, such as the diffusion term in reacting flows and homogenous mixing term in stirred reactors. A chemical explosive mode (CEM) is a chemical mode associated with an eigenvalue λ_e that has a positive real part. The eigenvalue λ_e and chemical Jacobian $\mathbf{J}$ are related by

$$\lambda_e = \boldsymbol{b}_e\cdot\mathbf{J}\cdot\boldsymbol{a}_e \tag{2}$$

where $\boldsymbol{a}_e$ and $\boldsymbol{b}_e$ are right and left eigenvectors, respectively, associated with the CEM. The CEM is a chemical property of a local mixture and indicates the propensity of a mixture to ignite if the mixture is isolated [19], i.e., when $\boldsymbol{s}=0$.

The utility of CEMA for flame diagnostics is demonstrated in Fig. 1, which shows the temperature profiles in homogeneous auto-ignition at various initial temperatures and 1-D freely propagating premixed flames of *n*-dodecane/air at different equivalence ratios. It is seen from Fig. 1a and b that the positive λ_e is present in the pre-ignition mixtures, and is absent in the post-ignition mixtures. Therefore, zero-crossing of λ_e indicates the ignition point in auto-ignition and the reaction front location in a propagating premixed flame.

2.2. An approximate CEMA formulation

Because the computational cost of eigen-analysis is a cubic function of the number of variables, CEMA may not be feasible to be performed on-the-fly for diagnostics of 3-D flame simulations when large chemical kinetic models are involved. To address this difficulty, an approximate CEMA formulation is developed in the present study to avoid the expensive eigen-decomposition.

To obtain an explicit formulation to approximate the CEM eigenvalue, Eq. (2) is decomposed into the contribution from each reaction as

$$\begin{aligned}\lambda_e =& \boldsymbol{b}_e\cdot\sum_{r=1}^{I}\mathbf{J}_r\cdot\boldsymbol{a}_e = \sum_{r=1}^{I}(\boldsymbol{b}_e\cdot\mathbf{J}_r\cdot\boldsymbol{a}_e)\\ =& \sum_{r=1}^{I}\left(\boldsymbol{b}_e\cdot\boldsymbol{\nu}_r\cdot\frac{\partial\Omega_r}{\partial\boldsymbol{c}}\cdot\boldsymbol{a}_e\right) = \sum_{r=1}^{I}\lambda_r\\ \frac{\partial\Omega_r}{\partial\boldsymbol{c}} =& \left[\frac{\partial\Omega_r}{\partial c_1},\frac{\partial\Omega_r}{\partial c_2},\ldots,\frac{\partial\Omega_r}{\partial c_{N_s}}\right], \quad \boldsymbol{\nu}_r = [\nu_{1,r},\nu_{2,r},\ \ldots,\ \nu_{N_s,r}]^T\end{aligned} \tag{3}$$

where $\mathbf{J}_r$ is the contribution to $\mathbf{J}$, λ_r is the contribution to λ_e, Ω_r is the reaction rate, of the rth reaction, N_s is the total number of species, I is the total number of reactions, c_k is the mole concentration of the kth species, and $\nu_{k,r}$ is the stoichiometric coefficient of the kth species in the rth reaction. A reaction is unimportant to the CEM if $|\lambda_r/\lambda_e|<\varepsilon$, where ε is a user-specified threshold, say 0.1. The remaining terms in Eq. (3) can be further related to the reaction timescales as

$$\lambda_e \approx \sum_{r=1}^{I_r}\lambda_r = \sum_{r=1}^{I_r}\frac{\alpha_r}{\tau_r} \tag{4}$$

where τ_r is the timescale of the rth reaction defined by Lam [23], α_r is a coefficient defined as $\alpha_r=\lambda_r\tau_r$, and I_r is the number of important reactions retained. The reaction timescale τ_r can be analytically evaluated as

$$\tau_r \equiv \left|\sum_{k=0}^{N_s}\frac{\partial\Omega_r}{\partial c_k}\nu_{k,r}\right|^{-1}. \tag{5}$$

In the present study, a series of 0-D calculations of steady-state perfectly stirred reactors (PSRs) are performed and the exact λ_r's and τ_r's are computed for the retained reactions. The coefficients α_r's are computed from the exact λ_r's and τ_r's, and then tabulated as functions of the mixture fraction and a progress variable defined as

$$C = (Y_{CO}+Y_{CO_2})/(Y_{CO}+Y_{CO_2})^{eq}. \tag{6}$$

PSRs are chosen for sampling because the approximate CEMA formulation obtained from PSR solutions, which include ignition, extinction and strongly burning flames, overall agrees well with the original CEMA compared with that obtained based on auto-ignition or 1-D freely propagating premixed flames alone. However, it is noted that PSR is by no means the only feasible reactor to provide sample reaction states for the development of reduced CEMA formulations.

2.3. Flame configuration and computational setup

The target flame in the present study is the Spray A (*n*-dodecane) flame of the engine combustion network (ECN) [24], with experimental data taken from a constant volume chamber at engine relevant conditions. The detailed experiment setup can be found in the literature [25,26], while the important flame conditions are summarized in Table 1.

The Spray A flame simulations are performed using the CFD code CONVERGE 2.3 [27,28], The computational setup is discussed

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