

Novel Tabulated Combustion Model Approach for Lifted Spray Flames with Large Eddy Simulations

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ABSTRACT

In this work, a turbulent combustion model is developed for large eddy simulation (LES) using a novel flamelet tabulation technique based on the framework of the multi-flamelet representative interactive flamelet (RIF) model. The overall aim is to develop a detailed model with elaborate chemistry mechanisms, LES turbulence models and highly resolved grids leveraging the computational cost advantage of a tabulated model. A novel technique of implementing unsteady flamelet libraries by using the residence time instead of the progress variables is proposed. In this study, LES of n-dodecane spray flame is performed using the tabulated turbulent combustion model along with a dynamic structure subgrid model. A high-resolution mesh is employed with a cell size of 62.5 microns in the entire spray and combustion regions. This model is then validated against igniting n-dodecane sprays under diesel engine conditions. For these constant volume combustion cases, 4-dimensional flamelet libraries based on scalar dissipation rate, residence time, mixture fraction variance and filtered mixture fraction are generated using a highly scalable parallel code. The flamelet libraries are generated using a 106-species and 420-reactions chemistry mechanism for n-dodecane. The transient flame development and the grid dependency shown by the tabulated model are analyzed. The results from the model show excellent agreement with the experimental measurements for ignition delay and flame liftoff across a wide range of ambient temperature conditions. The tabulated combustion modeling approach is also shown to have better agreements with the experiments than the homogenous reactor approach (typically used in the engine modeling community), while the computational expenses were significantly lower.

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INTRODUCTION

With the recent improvement in computational capabilities and the development of fast solvers [1], high-fidelity computational fluid dynamics (CFD) techniques like large eddy simulation (LES) have become viable for diesel engine applications [2]. In LES, the larger scales, which are hypothesized to carry the bulk of the turbulent kinetic energy, are fully resolved and the effects of the smaller scales are modeled. Chemical reactions occur at scales smaller than the scales resolved by LES and hence the effect of chemistry has to be modeled through the use of turbulence-chemistry interaction (TCI) models. This is one of the significant challenges in using LES for engine flows. Several TCI models have been used in the literature for diesel engine applications. These include flamelet models [3, 4], conditional moment closure models [5] and transported probability density function (PDF) models [6]. It is also a common practice in engine modeling community to neglect TCI modeling and use perfectly stirred reactor (PSR) models [7, 8], which assume that the chemical scales are fully resolved. The main aim of this work is to investigate novel flamelet tabulation strategies for non-premixed spray flames with detailed chemistry.

Flamelet-based TCI models are based on the assumption that the Damkohler number of the flow is high, which implies that chemical reactions occur in extremely thin regions (referred to as flamelets) and the effect of turbulence is to wrinkle and/or thicken these flamelets. Under these conditions, the governing equations for energy and species mass fractions can be transformed from the physical space to the one-dimensional mixture fraction (a coordinate normal to the flame surface) space, and these transformed set of equations are termed as the flamelet equations. In the representative interactive flamelet (RIF) approach, the flamelet equations are solved at each time step and the solutions are mapped back into the physical space. This approach is highly accurate because it does not make any additional assumptions apart from the flamelet assumption, and can also track the history effects on the flamelets resulting from unsteady scalar dissipation rates. However, the RIF model with multiple flamelets is computationally expensive as it involves solving a set of partial differential equations for each flamelet at every time step followed by a presumed PDF integration in each cell. The alternative approach, which is more computationally feasible, involves solving the flamelet equations prior to the CFD simulation and tabulating the solution in terms of a low-dimensional manifold. However, the

solution can depend on the choice of this manifold. This class of models include flamelet generated manifold (FGM) models [4] and flamelet progress variable (FPV) models [9].

The tabulated flamelet approaches, such as the FGM and FPV models, involve the use of a progress variable (c), which characterizes the extent of the transition of the flamelet from the mixed unburned state to the fully burned equilibrium state. The progress variable is traditionally defined either in terms of the temperature or in terms of the major products, such as CO, CO₂ and H₂O. However, this definition may not be ideal when the flamelet models are used with highly detailed chemistry that can involve species with highly different time scales, and thus the results can be influenced by the choice of the progress variable [10]. Kundu et al. [11] proposed a novel flamelet tabulation technique without the use of progress variables by utilizing the residence time along with multiple flamelet injection. They demonstrated the applicability of the model in a RANS framework and showed that the predictions approached the accuracy of the RIF approach but with a significantly lower computational expense. The objective of this work is to apply this procedure for an LES framework and demonstrate its accuracy and for predicting the ECN Spray A, a spray flame under diesel engine conditions. In the next section, the novel tabulated flamelet model approach will be described briefly.

This will be followed by a description of the LES computational setup. The results from the model will then be described including grid sensitivity, transient flame development, and the effect of ambient temperature. The results are also compared with a widely used multi-zone PSR approach and the accuracy and speedup of these two models will be discussed.

TABULATED FLAMELET MODEL FORMULATION

The details of the proposed turbulent combustion model, which will be referred to as the tabulated flamelet model (TFM), will be briefly discussed in this section. More details are available in Kundu et al. [11]. TFM is based on the flamelet assumption - chemical reactions are localized in infinitesimal thin regions known as flamelets and the effect of turbulence is to locally wrinkle and stretch these flamelets. The computational expense is reduced by parametrizing the flamelet in terms of a low dimensional manifold consisting of 4 variables: filtered mixture fraction, mixture fraction variance, filtered scalar dissipation rate, and residence time.

Flamelet Equations

When the transport equations for the species mass fractions and energy are transformed into the mixture fraction space (based on the flamelet assumption [12]), the resulting equations are termed as the flamelet equations which are shown below.

$$\rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i \quad (1)$$

$$\begin{aligned} \rho \frac{\partial T}{\partial t} - \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \rho \frac{\chi}{2} \left[\sum_i \left(\frac{C_{p,i}}{Le_i} \frac{\partial Y_i}{\partial Z} + \frac{\partial C_{p,i}}{\partial Z} \right) \right] \frac{\partial T}{\partial Z} \\ = \frac{1}{C_p} \left(\frac{\partial P}{\partial t} - \sum_i \dot{\omega}_i h_i \right) \end{aligned} \quad (2)$$

In Eq. (1) and (2), Y_i is the mass fraction of species i , T is the temperature, ρ is the density, Z is the mixture fraction, χ is the scalar dissipation rate, and $\dot{\omega}_i$ is the chemical source term of species i . In the present LES work, the filtered scalar dissipation rate is modeled based on Tillou et al. [13] as:

$$\tilde{\chi} = \chi_{res} + \chi_{sgs} = 2D|\nabla \tilde{Z}|^2 + 2\frac{D_t}{\Delta^2} Z_v, \quad (3)$$

where D is the molecular diffusivity of the mixture, D_t is the turbulent diffusivity, Δ is the grid size and Z_v is the mixture fraction variance. This model for filtered scalar dissipation rate was implemented into the CFD code in the form of a user defined function. The functional dependence of χ on Z is parametrized in terms of its stoichiometric value based on the following profile recommended by Peters [14].

$$\chi(Z) = \chi_{st} \frac{\exp[-2(\text{erfc}^{-1}(2Z))^2]}{\exp[-2(\text{erfc}^{-1}(2Z_{st}))^2]} \quad (4)$$

In Eq. (4), st refers to the stoichiometric condition and χ_{st} is the stoichiometric scalar dissipation rate. By solving the flamelet equations (Eqs. (1-2)) using the scalar dissipation rate profile of Eq. (4), the species mass fractions are obtained as a function of Z , χ_{st} , and the time, t , i.e., $Y_i = Y_i(Z, \chi_{st}, t)$. The effect of turbulence on the flame structure is represented by integrating the species mass fractions using a beta PDF, which is a function of the filtered mixture fraction ($\tilde{Z}$) and the mixture fraction variance (Z_v). Thus, the species fractions for the TFM is a function of four independent variables.

$$\tilde{Y}_i = \tilde{Y}_i(\tilde{Z}, Z_v, \chi_{st}, t) \quad (5)$$

This solution is then pre-tabulated and used during the LES simulation.

Multiple Flamelet Injection

In the TFM approach, the use of multiple flamelets suggested by Barths et al. [15] is employed. In this approach, multiple flamelets are introduced sequentially into the computational domain through the spray injection. The different flamelets are tracked through the solution of marker equations, given by:

$$\frac{\partial(\tilde{\rho}\tilde{Z}_l)}{\partial t} + \frac{\partial(\tilde{\rho}\tilde{u}_l\tilde{Z}_l)}{\partial x_l} = -\frac{\partial(\tilde{\rho}\tilde{u}_l''\tilde{Z}_l'')}{\partial x_l} \quad (6)$$

These markers satisfy the following condition:

$$\tilde{Z} = \sum_{l=1}^n \tilde{Z}_l, \quad (7)$$

where n is the number of flamelets. The scalar dissipation rate for each flamelet is determined as:

$$\widehat{\chi}_{st}(l) = \frac{\int \frac{\tilde{Z}_l}{\tilde{Z}} \bar{\rho} \tilde{\chi}_{st}^2 \tilde{P}(Z_{st}) dv}{\int \frac{\tilde{Z}_l}{\tilde{Z}} \bar{\rho} \tilde{\chi}_{st}^2 \tilde{P}(Z_{st}) dv}, \quad (8)$$

where $\widehat{\chi}_{st}$ is the spatially averaged stoichiometric scalar dissipation rate.

Table Lookup

In each computational cell, the species mass fractions are obtained as the sum of the contributions of all n flamelets. The contribution of flamelet l is obtained using the table lookup given by:

$$\tilde{Y}_{l,i} = \tilde{Y}_{l,i}(\tilde{Z}_l, Z_v, \widehat{\chi}_{st}(l), t_l), \quad (9)$$

where t_l is the residence time of flamelet l . The residence time is here defined as the time that the flamelet has resided in the computational time since its injection. So, at the same physical time, the flamelets injected earlier in the simulation will have larger residence time than the flamelets injected later. The final species mass fractions are then obtained as weighted averages of all flamelets as:

$$\tilde{Y}_i = \sum_{l=1}^n \frac{Z_l}{\tilde{Z}} \tilde{Y}_{l,i} \quad (10)$$

The schematic in Figure 1 shows the integration of TFM into the CFD code. The CFD code solves for the continuity, momentum, energy and mixture fraction equations. A tabulated 4D data set is generated *a priori* for each simulation with a given range of variables. The flamelets are divided based on injected fuel mass and a mass-weighted fraction of the fuel that are being injected were tracked using marker equation (Eq. (6)). The stoichiometric scalar dissipation rates of each flamelet are calculated using Eq. (8). At every time-step iteration, $\widehat{\chi}_{st}(l)$, and residence time, t_p , of each flamelet are known. A 4D linear interpolation scheme is then used to determine the species mass fractions for each cell. These species mass fractions are then calculated for all the remaining flamelets iteratively and the final mass fraction at any cell is given by Eq. (10).

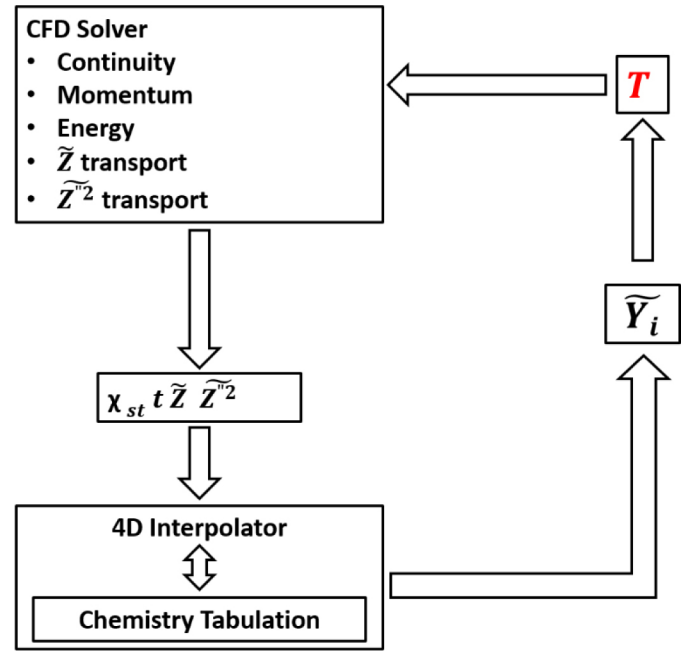


Figure 1. Schematic showing the integration of TFM into the CFD code

COMPUTATIONAL SETUP

In this work, the TFM is integrated with the commercially available CFD code Converge [16]. The capability of the TFM model is demonstrated using LES of Spray A from the Engine Combustion Network (ECN) [17]. Spray A is characterized as an n-dodecane spray injected into a constant volume combustion chamber wherein the evolution of the spray flame is studied. In the present study, the injection pressure is chosen to be 150 MPa, the ambient oxygen concentration is chosen to be 15%, and the ambient density is chosen to be 22.8 kg/m³ which is the typical Spray A condition. Ambient temperature range from 800 K to 1100 K is simulated to further test the TFM code. The experimental conditions simulated in this study are summarized in Table 1.

Converge solves the gas phase equations using an Eulerian approach and the dispersed phase using a Lagrangian-parcel approach. Table 2 summarizes the spray and subgrid models employed in the present study. More details about the setup are described in detail in previous publications from our group [7, 8]. The spray submodels employed in the current work have been validated by Senecal et al. [18] and Xue et al. [19]. The chemical kinetics are modeled using a 103-species, 370-reaction mechanism [20] for n-dodecane. A schematic of the computational domain is shown in Fig. 2. Adaptive mesh refinement is employed such that the entire spray and flame regions are resolved using a fine grid, whereas a coarser grid is employed outside the region of interest. For the TFM model, 20 flamelets were employed for the simulations. Kundu et al. [11, 21] performed a sensitivity study on the effect of the number of flamelets for RANS calculations and showed that 20 flamelets was sufficient for the Spray A condition. Although this analysis was not repeated for LES, 20 flamelets is assumed to be sufficient for all the cases simulated in this study with the TFM model. Kundu et al. [11, 21] performed a sensitivity study on the resolution of the tabulated dataset for RANS calculations and showed that the optimum is 20 points in χ_{st} , 28 points in χ_{sp} , 21 points in t , 120 points in $\tilde{Z}$, and 21 points in $\tilde{Z}^2$. This