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## Chemical Engineering Science



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### An evaluation of the assumptions of the flamelet model for diesel combustion modeling



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#### HIGHLIGHTS

The validity of flamelet model evaluated for diesel combustion.

Dependence of scalar dissipation rate on time and mixture fraction.

Simple ad hoc modification to the flamelet model.

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#### ABSTRACT

Flamelet-based models are widely used to model turbulence-chemistry interaction in Reynolds-Averaged Navier–Stokes (RANS) simulations and Large Eddy Simulations (LES). In this study, one-dimensional laminar and two-dimensional Direct Numerical Simulations (DNS) of reacting mixing layers are used to assess the validity of flamelet models in turbulent diesel jets. The pressure and initial temperature are chosen to be similar to those found in diesel engine combustion chambers at the end of compression. The validity of the flamelet model is first evaluated by comparing the flame development predicted by DNS with that predicted by solving the unsteady flamelet equations. It is shown that there are significant differences in the temperature profiles during the flame development following autoignition. This difference in the unsteady flame development can be a source of error in predicting ignition and flame development. The difference is attributed to the fact that in flamelet models, the dependence of scalar dissipation rate,  $\chi$ , on the mixture fraction, Z, is assumed to have a constant functional relationship, usually an error function profile, which remains unchanged during the flame development process. The DNS results show that the chemical reactions cause significant increase in the local scalar dissipation rate near the flame. This increase leads to higher diffusion rates for the active radicals near the flame and thus faster flame development. It was shown that solving the unsteady flamelet equations using the scalar dissipation rate profiles obtained from one-dimensional direct simulations lead to less than 5% error in the temperature profiles during the flame development. Since this approach is not computationally feasible for practical applications, an ad hoc modification of the error function profile employed in generating flamelet libraries is proposed for the scalar dissipation rate to account for the chemical reactions and the results show an improved performance compared to the traditional flamelet approach.  $\odot$  2015 Elsevier Ltd. All rights reserved.

#### 1. Introduction

Reynolds-averaged Navier–Stokes (RANS) solvers are commonly employed to model combustion in diesel engines. With increasing computational power, large-eddy simulations (LES) are also becoming viable [\(Rutland, 2011\)](#page--1-0). The biggest challenge in using LES for these applications involves the accurate modeling of turbulence-chemistry interactions. In the LES governing equations, the effect of turbulence on chemistry appears as the filtered reaction rate term, which can be thought of as the convolution of the local and instantaneous reaction rate with the joint probability density function (PDF) of the scalar variables at that point and time. In prior work, flamelet models with á-priori PDFs, conditional moment closure (CMC) models with á- priori PDFs, and transported PDF or filtered density function (FDF) models have

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been employed for modeling the reaction rate [\(Peters, 2000;](#page--1-0) [Veynante and Vervisch, 2002](#page--1-0); [Bajaj et al., 2013;](#page--1-0) [Pei et al., 2013;](#page--1-0) [Bhattacharjee and Haworth, 2013\)](#page--1-0).

For turbulent non-premixed combustion, flamelet-based models are attractive when the combustion occurs in reaction zones that are smaller than the Kolmogorov scale. Under these conditions, the unsteady flamelet equations are derived by assuming that the flame is locally one-dimensional in the mixture fraction (Z) space. The evolution of the temperature and species mass fractions are then governed by

$$
\rho \frac{\partial \phi}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 \phi}{\partial Z^2} + \dot{\omega}_{\phi},\tag{1}
$$

where  $\rho$  is the density,  $\phi$  is a vector representing the set of all reactive scalars, which includes the temperature and mass fractions of all the species, and is the corresponding source term due to chemical reactions. The implicit assumption is made that all the species have the same molecular diffusivities. This is a reasonable assumption for diesel flames. The symbol  $\gamma$  represents the instantaneous scalar dissipation rate defined as

$$
\chi = 2D|\nabla Z|^2,\tag{2}
$$

where *D* is the molecular diffusivity.  $\chi$  is a function of the mixture fraction Z and time, t.

In most implementations of the flamelet model, it is assumed that the functional form of the dependence of  $\chi$  on Z follows an error function profile ([Peters, 2000;](#page--1-0) [Mukhopadhyay and Abraham,](#page--1-0)



Fig. 1. Schematic of the UFPV model implementation as a turbulence/chemistry interaction model in LES.



[2012](#page--1-0)) that is assumed to be independent of time, i.e.,

$$
\chi = \chi_{\rm st} \frac{\exp\left\{-2\left[\,erfc^{-1}(2Z)\right]^2\right\}}{\exp\left\{-2\left[\,erfc^{-1}(2Z_{\rm st})\right]^2\right\}}.\tag{3}
$$

The expression in Eq.  $(3)$  is exact for the case of opposed diffusion flames with constant density and diffusivity [\(Peters, 1983\)](#page--1-0). [Peters \(1983](#page--1-0)) showed that Eq. (3) is also exact if  $\rho^2D$ , where  $\rho$  is the density and  $D$  is the molecular diffusivity, remains constant with respect to time. The validity of this assumption will be assessed in [Section 3](#page--1-0). By using Eq. (3), the value of the scalar dissipation rate at any Z can be related to its value at the stoichiometric mixture fraction,  $\chi_{st}$ . Here, a fundamental problem in the implementation becomes obvious. The molecular diffusivity D is a function of temperature. In a flame evolving after local ignition at some value of Z, D will vary with Z and time. The model does not account for this effect. Yet, the model has been employed to model autoigniting jets [\(Bajaj et al., 2013;](#page--1-0) [Ihme et al., 2005](#page--1-0); [Ihme and](#page--1-0) [Pitsch, 2008;](#page--1-0) [Ihme and See, 2010\)](#page--1-0). There have been a few other approaches in modeling the scalar dissipation rate profile in the flamelet equation. [Blanquart and Pitsch \(2005](#page--1-0)) employed a timevarying profile for the scalar dissipation rate which had a quadratic dependence on the mixture fraction. They showed that the fluctuations in scalar dissipation rate are very important in determining ignition. [Pitsch et al. \(2000\)](#page--1-0) also employed a time-varying



Fig. 3. Initial fuel mass fraction as a function of the y-coordinate.



Fig. 2. (a) The initial mixture fraction field in the computational domain for the 2-D turbulent simulation. (b) Temperature profiles in the computational domain for the 2-D turbulent simulation at 0.5 ms.

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