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An equivalent dissipation rate model for capturing history effects in non-premixed flames

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ABSTRACT

The effects of strain rate history on turbulent flames have been studied in the past decades with 1D counter flow diffusion flame (CFDF) configurations subjected to oscillating strain rates. In this work, these unsteady effects are studied for complex hydrocarbon fuel surrogates at engine relevant conditions with unsteady strain rates experienced by flamelets in a typical spray flame. Tabulated combustion models are based on a steady scalar dissipation rate (SDR) assumption and hence cannot capture these unsteady strain effects; even though they can capture the unsteady chemistry. In this work, 1D CFDF with varying strain rates are simulated using two different modeling approaches: steady SDR assumption and unsteady flamelet model. Comparative studies show that the history effects due to unsteady SDR are directly proportional to the temporal gradient of the SDR. A new equivalent SDR model based on the history of a flamelet is proposed. An averaging procedure is constructed such that the most recent histories are given higher weights. This equivalent SDR is then used with the steady SDR assumption in 1D flamelets. Results show a good agreement between tabulated flamelet solution and the unsteady flamelet results. This equivalent SDR concept is further implemented and compared against 3D spray flames (Engine Combustion Network Spray A). Tabulated models based on steady SDR assumption under-predict autoignition and flame lift-off when compared with an unsteady Representative Interactive Flamelet (RIF) model. However, equivalent SDR model coupled with the tabulated model predicted autoignition and flame lift-off very close to those reported by the RIF model. This model is further validated for a range of injection pressures for Spray A flames. The new modeling framework now enables tabulated models with significantly lower computational cost to account for unsteady history effects.

1. Introduction

Turbulent non-premixed flames are subject to unsteady strain effects, also referred to as history effects. The influence of unsteady strain on flames with respect to ignition, extinction, and species concentration has been the focus of numerical and experimental work by many researchers in the past decades. Peters and William [1] discussed a flame stabilization mechanism for non-premixed counter flow diffusion flames (CFDF) based on quenching limits of flamelets and their dependence on scalar dissipation rate (SDR). This was also supported by findings of Mastorakos et al. [2]. Egolfopoulos et al. [3] numerically studied 1D CFDF with periodic strain rates. The flame response was quasi-steady for very high and very low frequencies. However, the intermediate frequencies showed a phase shift between the oscillations and the flame response. Similarly, Kistler et al. [4] carried out experimental and numerical study of CFDFs and observed that for very low and high frequencies in strain oscillations, the behavior was quasi-steady. Extinction was not observed for very high frequencies with peak strain values beyond quenching limits. Im et al. [5] studied CFDFs under oscillating strain with similar conclusions. It was suggested that as the strain rate increases beyond the extinction limits, the flamelet needs some time to respond to this rapid change. If the time scale of oscillation is not long enough then these high strain rates are not sufficient for the flame to extinguish. Similar results were observed by Brown et al. [6]. Barlow et al. [7] studied the effect of a temporal step change (sudden decrease) of strain on flamelets experimentally as well as numerically using the steady flamelet assumption. The results showed that the steady flamelet assumption over-predicted the OH and CO species concentrations. Overall, these studies show that the flame response, including its ignition characteristics depends not only on scalar dissipation rate, but also on its history.

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The Representative Interactive Flamelet (RIF) model solves the unsteady flamelet equations at each time-step, thus accounting for the history effects in flamelets. These models have been implemented in a number of simulations over a wide range of spray combustion regimes from HCCI (homogeneous charge compression ignition) to diesel combustion [8–16]. However, the need for multiple flamelets and the online solution of flamelet equations at each time step have resulted in these models being computationally expensive and prohibitive for high-fidelity engine simulations. A less expensive method is to solve the flamelet equations *a priori*, for a range of conditions and tabulate the species as a lower dimensional manifold. The unsteady nature of chemistry is accounted in these manifolds through the implementation of a progress variable. This category of tabulated flamelet models include Flamelet Progress Variable (FPV) [17,18], Unsteady Flamelet Progress Variable (UFPV) [19–21] and Flamelet Generated Manifolds (FGM) [22–25].

Large chemistry mechanisms necessary for accurate simulation of hydrocarbon fuels lead to high computational costs. Efforts have been directed towards speeding up stiff chemical kinetics calculations [26]. Tabulated flamelet models have been used extensively and have successfully reduced computational costs in practical combustion problems while incorporating high fidelity chemistry mechanisms. The progress-variable type unsteady models, which can take into account unsteady chemical kinetics, however, cannot account for the effect of unsteady strain rate history. The lower dimensional manifolds are generated for a range of SDRs by solving the flamelet equations. During these computations the SDR of each flamelet equation is kept constant. This is referred to as the steady strain assumption and implies that the flamelet can instantaneously adjust to the local scalar dissipation rate. As a result, the resulting model cannot capture the effect of unsteady strain rate history of a flamelet. Various approaches that attempt to incorporate unsteady effects in recent years have been primarily restricted to oscillatory strain for flames under atmospheric pressures. Haworth et al. [27] studied the effects of time varying strain rates on flamelets and suggested a formulation to calculate an equivalent strain based on the history of the strain rate. The equivalent strain was then coupled with a tabulated steady flamelet library. It needs to be investigated how these methods can be applied towards unsteady tabulated flamelet libraries. Cuenot et al. [28] proposed the idea of calculating an equivalent strain based on the history of a flamelet. This formulation and its validation was based on single-step chemistry and a single time scale associated with the frequency of strain rate oscillations. For chemistry involving multiple species, an equivalent strain needs to be calculated for each species. Delhaye et al. [29] developed a framework to incorporate unsteady effects in FGM based on 2D (with 2 controlling variables) and 3D (with 3 controlling variables) manifold. This was used to predict species for a flamelet subject to periodic strain rate and compared with detailed unsteady simulations using GRI 3.0 chemistry mechanism [30] for methane. The 3D manifold resulted in better comparisons with the unsteady periodic strain rate simulation. In contrast to the 2D manifold, this did not exhibit a phase shift relative to the unsteady simulations. The work was further extended to extinction limits by Delhaye et al. [31].

Studies based on periodic strain rate oscillations may be relevant to a number of applications. However, these findings cannot be generalized to other configurations, such as the configuration of interest here, which corresponds to spray flames under diesel-like conditions [14,15]. More importantly, it is essential to capture the onset of autoignition and the transition to lifted flames. A strong correlation between these parameters and pollutant formation has been established for diesel flames. The scalar dissipation rates in spray flames experience much larger gradients and decay exponentially over a short period of time, as the flamelet like structures move away from the nozzle, as shown in previous studies by our group [14]. Understanding the unsteady history effects in these flames that lead to the onset of autoignition or extinction behavior is a principal motivation for this work. More importantly, the ability to exploit a tabulation scheme for these effects as an alternative strategy to *in situ* unsteady flamelet simulations may provide a significant computational saving, given the chemistry complexity associated with practical fuels.

The objectives of this work are two-fold. The first objective is to quantify these history effects and to investigate if these effects are significant for diesel injection applications. The second objective is to develop a model that can incorporate these effects, and implement a tabulation approach for these effects to overcome the inherent computational cost of *in situ* unsteady flamelet simulations. Strain rates in flamelet computations are best represented through an equivalent contribution in mixture fraction space, the SDR, which is normally identified with the dissipation rate at stoichiometric mixture conditions. In the following sections, we first attempt to quantify the contribution of dissipation rate and its temporal variations on the autoignition process and subsequent high-temperature combustion (Section 2). Then we propose an equivalent dissipation rate model that is designed to capture dissipation rate histories as presented in Section 2.4. Finally, this concept is validated for 1D flamelet calculations (Section 3), and 3D RANS simulations are presented and discussed in Section 4. Conclusions are presented in Section 5.

2. Evaluation of history effects in 1D flamelets under diesel-relevant conditions

To understand the role of unsteady dissipation rates on the evolution on autoignition and the formation of non-premixed flamelets, 1D unsteady flamelet simulations are carried out. The same simulations will provide the database to construct the equivalent dissipation rate model discussed below. The flamelet problem is set up for high pressure engine relevant conditions with n-dodecane as the fuel surrogate for diesel. The pressure is set to 60 bar and oxidizer stream is diluted with CO_2 and H_2O as per engine relevant Sandia Spray A exhaust gas re-circulation (EGR) conditions [32]. The ambient oxidizer temperature is set at 900 K. The stoichiometric scalar dissipation rate for the flamelet is varied linearly over time in the first part of the 1D study. The flamelets are initialized at unburnt conditions and the unsteady igniting flamelet problem is solved up to 0.63 ms. The 106 species n-dodecane chemistry mechanism with 420 reactions is used to model the chemical kinetics in the unsteady flamelet and all the other 3D CFD simulations [33].

In the section below, we study a 1D counter-flow diffusion flame subject to time-varying scalar dissipation rates with 3 different modeling approaches. They include (1) the unsteady flamelet model, which is the most accurate, and also the most expensive method for determining the effects of time-evolving dissipation rates, (2) the steady SDR flamelet approach, which looks up the solution of the current SDR without accounting for its time history, and (3) the equivalent SDR model, which is proposed within the context of the present work.

2.1. Unsteady flamelet model

In this model, the following unsteady flamelet equations are solved:

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