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Conditional moment closure modelling for HCCI with temperature inhomogeneities

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Abstract

This paper presents an approach for modelling combustion in homogeneous charge compression ignition (HCCI) conditions based on the first order conditional moment closure (CMC) method. The model is implemented into the open source C++ computational fluid dynamic (CFD) code known as OpenFOAM. Direct numerical simulations (DNSs) are used to evaluate the performance of the CFD-CMC solver. In the two-dimensional (2D) DNS cases, ignition of a lean *n*-heptane/air mixture with thermal inhomogeneities is simulated for nine cases, with two different mean temperatures and several different levels of thermal stratification. Results from the CFD-CMC solver are in excellent agreement with the DNS for cases which exhibit a spontaneous sequential ignition mode of combustion whereas for the cases in which a mixed mode of deflagration and spontaneous ignition exists, the CMC underpredicts the ignition delay. Further investigation using the DNS data demonstrates that this discrepancy is primarily attributed to the first order closure assumption. Conditional fluctuations are found to be more significant in the case with deflagrations. Further analysis of the DNS shows that scalar dissipation fluctuations are the cause of conditional fluctuations.

Keywords: Conditional moment closure; Thermal stratification; HCCI; *n*-Heptane

1. Introduction

Due to its potential for high efficiencies and low emissions, homogeneous charge compression ignition (HCCI) combustion has been a topic of considerable interest [1]. Two of the main challenges in developing HCCI engine are controlling the auto-ignition timing, particularly during transients, and limiting the rate of heat release, particularly at high loads [2]. Because of the importance of temperature in autoignition

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processes, thermal stratification has a huge impact on both the timing and rate of heat release, as well as being an important influence on pollutant formation [3–21]. Detailed, laser-based experiments have shown that temperature fluctuations always occur in HCCI engines; they have identified several sources for these fluctuations and contributed significantly to how they affect the process of ignition in the engine [1–9].

To further understand thermal stratification effects on ignition and combustion in HCCI, detailed direct numerical simulation studies (DNSs) have been carried [10–16]. However, DNS methods are not affordable as a design tool, which motivates the development of computationally cheaper models, such as flamelet-based models [17–19], probability density function models [20] or multi-zone approaches [4,21].

In the present study, a combustion model based on the concept of conditional moment closure (CMC) [22] is developed to model ignition under conditions of HCCI combustion. The background and motivation to this is outlined below. Klimenko and Bilger [22] developed the CMC transport equations for non-premixed turbulent combustion. The main concept of the CMC approach is to significantly reduce the error of closure of mean reaction rates by conditioning on a variable upon which the thermochemical state mainly depends and which, preferably, has a transport equation that is readily closed. The CMC method has been successfully applied to various non-premixed combustion systems [23–27]. However, relatively fewer studies have been performed using CMC to model premixed combustion [28–30]. The main challenge in the context of premixed flames is to choose an appropriate conditioning variable. In non-premixed flames, mixture fraction is usually chosen as a conditioning variable, whereas a variety of scalars have been proposed for premixed flames [28,29,31].

HCCI is primarily a kinetically controlled mode of combustion, which is markedly different from spark and diesel engine combustion modes that involve mixing as a key rate limiting process. Since the charges in HCCI engines are nearly homogeneous, they tend to ignite almost simultaneously and once ignited burn rapidly, so that there is very little time for mixing between unburned, burning and burned regions. As a result, the combustion behaviour is determined mainly by the thermochemical state prior to ignition. Therefore, with an appropriate choice of conditioning variables to represent this state, conditional fluctuations are expected to be small. In general, fluctuations of the state are likely to be due to heat transfer leading to temperature fluctuations, imperfect fuel–air mixing leading to mixture fraction and temperature fluctuations, and imperfect residual-fresh gas mixing leading to fluctuations in temperature and oxygen fraction. This study considers only the case of temperature fluctuations. In this case, enthalpy (chemical plus sensible) is the natural choice of a conditioning variable, since it encapsulates the strong effect of temperature while also not having a source term that exhibits significant spatial variations, as this would result in a closure problem for the conditioning variable.

The structure of the paper is as follows. The CMC modelling is first introduced. The enthalpy-conditioned variables are solved in a spatially zero-dimensional domain which is two-way coupled to a CFD flow solver. The numerical method related to the structure of CFD-CMC solver is then presented. The model is validated using 2D DNS data which modelled constant volume ignition of a lean n-heptane/air mixture with temperature inhomogeneities presented by Yoo et al. [14]. Finally, reasons for the observed discrepancies between the CMC model and the DNS are analysed using the DNS data [14].

2. Conditional moment closure (CMC)

In the following, equations and definitions required to derive the premixed CMC equation will be given. Under the assumption of negligible radiation,[1] unity Lewis numbers, and low Mach number, the species transport equation is:

$$\rho \frac{\partial Y_\alpha}{\partial t} = -\rho v_j \frac{\partial Y_\alpha}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial Y_\alpha}{\partial x_j}\right) + \dot{\omega}_\alpha, \qquad (1)$$

and the enthalpy transport equation is:

$$\rho \frac{\partial h}{\partial t} = -\rho v_j \frac{\partial h}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial h}{\partial x_j}\right) + \frac{Dp}{Dt}, \qquad (2)$$

where Y_α is the mass fraction of species α, ρ is the density, h is the enthalpy, p is the pressure, v_j is the velocity in the x_j direction, and D is the molecular diffusivity, which is assumed to be equal to the thermal diffusivity.

A normalised scalar variable is defined as follows,

$$\theta(x,t) = \frac{h(x,t) - h_{min}(t)}{h_{max}(t) - h_{min}(t)},$$

where h_{min} and h_{max} correspond to minimum and maximum enthalpies in the computational domain, respectively, which are only a function of time.

The conditional mean and the Favre-conditional mean of a given quantity ϕ are shown with $\overline{\phi|_{\theta=\xi}}$ and $\langle \phi|_{\theta=\xi}\rangle$, respectively, where ξ is the sample space for normalised enthalpy. If

[1] Because of the low levels of soot formation, radiation is insignificant in typical HCCI engine operating conditions [32].

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