



Doubly conditional moment closure modelling for HCCI with temperature inhomogeneities

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Abstract

This paper presents a doubly conditional moment closure (DCMC) as an *a posteriori* predictive modelling tool for ignition of mixtures with large thermal stratification in homogeneous charge compression ignition (HCCI) conditions. Double conditioning is applied on enthalpy and its dissipation rate. The performance of the DCMC model is evaluated using a number of previously reported direct numerical simulations (DNSs) with various fuels. The DNSs modelled ignition of various lean homogeneous mixtures with a high level of temperature inhomogeneities. The selected cases exhibit a prevalence of deflagration mode of combustion as opposed to a spontaneous ignition-front mode, which has proven challenging for previous singly CMC. In all simulations, DCMC solver is run in a stand-alone mode with certain terms, such as the probability density functions of enthalpy and dissipation rate, being provided using the DNS input. The DCMC results are in a very good agreement with the DNS data, and are significantly improved compared with a singly conditional moment closure. A set of *a posteriori* DNS-DCMC tests is also performed to demonstrate importance of various terms in the doubly CMC equations. These tests first reveal that the effects of the cross dissipation and sources of enthalpy and dissipation rate (which lead to convective terms in conditional space) are insignificant and these terms can be safely neglected from the DCMC equations. The significance of this result is that the

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main unclosed models that would be needed for satisfactory results in a practical simulation of an engine would be the joint probability density function of enthalpy and its dissipation rate and the dissipation rate of dissipation rate.

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1. Introduction

Reducing formation of pollutants and optimising engine efficiency are key concerns in developing engine technologies. A possible solution, having potential for achieving high efficiency and low emissions, can be homogeneous charge compression ignition (HCCI). Using the HCCI concept nitrogen oxides (NO_x) and soot formation are suppressed by keeping the flame temperature below the formation threshold via overall lean mixtures. However, lack of a means to control the combustion phasing, especially during transients, and the high rate of pressure rise at high load conditions pose significant technical challenges [1]. Hence, HCCI is still in the phase of laboratory research and has not seen commercial success yet. Nevertheless, HCCI could well be effective in particular operating regimes and combined with other strategies where HCCI is too challenging.

Thermal stratification in an HCCI engine cylinder can reduce the pressure rise rate under high-load [1,2]. Effects of thermal stratification on the ignition process have been widely studied by direct numerical simulation (DNS) for various mixtures under HCCI conditions [3–8]. The DNS studies show that different combustion modes can be observed depending on the degree of thermal stratification [3–8]. Under low levels of thermal stratification, the spontaneous combustion mode is prevalent. However, under high thermal stratification conditions, gradients of ignition delay are sufficiently large to result in significant fraction of burning in premixed flames where conduction and diffusion effects become important, *i.e.* in a deflagrative mode of combustion.

In previous study [9], a model based on the first-order singly conditional moment closure (CMC) was developed to study HCCI combustion. The basic idea behind the CMC approach is that errors in the evaluation of the unclosed reaction source term can be significantly reduced if its evaluation is conditioned on another variable upon which the reaction rate mainly depends [10]. The CMC model for HCCI was evaluated using various sets of DNS data [4,5] with various levels of temperature fluctuations. It was found that the first-order singly CMC

model cannot predict the ignition process as well in conditions of large thermal stratification compared with low and medium stratification levels. In the former conditions, the deflagration mode is dominant and there is a strong correlation between dissipation fluctuations and conditional fluctuations of scalars (*e.g.* temperature and radical mass fractions) which are not considered in the first-order singly CMC model [9,11].

This paper makes an original contribution towards advancing combustion modelling under HCCI conditions, aiming to improve the performance at high stratification levels. There are various options for achieving this including higher order closures [10,12–16] or conditioning on multiple variables [17,18]. For example, a second-order closure is a possible extension of the first-order singly closure [10]. In second-order closures, using Taylor expansions, effects of species-species and temperature-species correlations are accounted for in the conditional reaction rates. However, an *a priori* study [19] revealed that the second-order conditional moment closure was not a promising solution for large stratifications. Second-order CMC is also computationally expensive, particularly for more realistic hydrocarbon fuels involving a chemistry mechanism with a large number of species. Alternatively, double conditioning of the reactive scalar transport equations can be used to improve the first-order singly conditional closure prediction [17,18,20–22]. By choosing a suitable second conditioning variable, the fluctuations around the doubly conditioned mean can be reduced in comparison with the singly conditioned case and then the first-order closure of the conditional chemical source term remains valid in which doubly conditioned reaction rate is a function of doubly conditioned species mass fraction and temperature.

An extension of the first-order singly CMC to include a second conditioning variable was initially proposed by Bilger [20] and it has been investigated for non-premixed flames in Refs. [17,18,21–23]. In earlier studies for non-premixed flames, mixture fraction was considered as the first conditioning variable while several second conditioning variables such as dissipation rate [21], sensible enthalpy [17,18] and a normalised mixture fraction-dependent temperature [22] have been proposed with varying degrees of success and

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