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Probability density function treatment of turbulence/chemistry interactions during the ignition of a temperature-stratified mixture for application to HCCI engine modeling

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Abstract

Homogeneous charge compression ignition (HCCI) engine technology promises to reduce NO_x and soot emissions while achieving high thermal efficiency. Temperature and mixture stratification are regarded as effective means of controlling the start of combustion and reducing the abrupt pressure rise at high loads. Probability density function methods are currently being pursued as a viable approach to modeling the effects of turbulent mixing and mixture stratification on HCCI ignition. In this paper we present an assessment of the merits of three widely used mixing models in reproducing the moments of reactive scalars during the ignition of a lean hydrogen/air mixture ($\Phi = 0.1$, $p = 41$ atm, and $T = 1070$ K) under increasing temperature stratification and subject to decaying turbulence. The results from the solution of the evolution equation for a spatially homogeneous joint PDF of the reactive scalars are compared with available direct numerical simulation (DNS) data [E.R. Hawkes, R. Sankaran, P.P. Pébay, J.H. Chen, Combust. Flame 145 (1–2) (2006) 145–159]. The mixing models are found able to quantitatively reproduce the time history of the heat release rate, first and second moments of temperature, and hydroxyl radical mass fraction from the DNS results. Most importantly, the dependence of the heat release rate on the extent of the initial temperature stratification in the charge is also well captured.

Keywords: Probability density function; HCCI; Mixing models

1. Introduction

Homogeneous charge compression ignition (HCCI) engine technology has received increasing attention in recent years due to its intrinsic benefits in terms of high efficiency and low NO_x and soot

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emissions [1,2]. However, unresolved issues include combustion phasing (i.e., the control of the start and duration of combustion), high carbon monoxide and unburnt hydrocarbon emissions, limited load-speed operating window, and transition to spark-ignited combustion at high loads [3]. Several strategies for mixture control have been devised and are currently being considered to help overcome these difficulties. These include diverse fuel injection schemes such as port fuel injection and single or multistage direct injection (DI or MDI), as well as external exhaust gas recirculation (EGR), variable valve timing, and variable compression ratio [4]. The technological solutions mentioned above aim at creating a well-calibrated near-homogeneous charge of fuel and air to control the ignition event. Also, hot residuals of combustion (either as external or internal EGR) are judiciously used to preheat the charge, thus affecting ignition delay time. In addition to stratification purposely introduced into the charge, heat loss to the walls and composition inhomogeneity that develop during ignition due to temperature stratification are also found to be significant.

As the in-cylinder conditions depart from the ideally homogeneous mixture charge, which becomes *stratified* in composition and/or temperature, turbulent mixing is found to play an increasingly important role in controlling the combustion event [5–7]. The interactions of turbulent fluid motion with chemical reactions constitute a great modeling challenge, which has been the subject of research in the turbulent combustion community for several decades [8]. Nevertheless, the inclusion of the effect of turbulent mixing on heat release rate and emissions is considered a necessary step to improve the predictive capabilities of current HCCI engine simulations, especially in the presence of temperature and composition inhomogeneities [4].

In order to better understand the ignition process under inhomogeneous conditions and to assess the relative importance of transport compared to chemical reactions, thus aiding modeling efforts, Chen et al. [9] and Hawkes et al. [10] performed a direct numerical simulation (DNS) study of autoignition of a lean hydrogen/air mixture with temperature stratification under typical HCCI conditions. In their parametric study, they observed a significant effect of temperature stratification on ignition timing as well as on heat-release-rate patterns. Increasing temperature stratification led to an advanced and smoother burn. Also, they showed that, under increasing temperature stratification, molecular diffusion of heat and chemical species becomes important, causing the coexistence of two ignition regimes: spontaneous ignition and diffusion-limited combustion (i.e., deflagration).

The choice of a lean hydrogen/air mixture for the DNS work was mainly dictated by the need to match computational requirements and available resources [9]. In fact, hydrogen/air combustion chemistry can be reasonably described with few chemical species and reactions, as opposed to hydrocarbon fuels. Notwithstanding the above-mentioned reasons related to computational requirements of the DNS simulation, hydrogen chemistry is relevant to hydrocarbon combustion, as hydrogen chemistry plays a key role in higher hydrocarbon oxidation. Furthermore, hydrogen may play an increasingly important role among fuels for automotive applications in the future due to desirable combustion characteristics such as zero tailpipe emissions of CO_2, particulates, and unburned hydrocarbons. Finally, hydrogen is also being considered as an alternative automotive fuel that could alleviate the exclusive role played by hydrocarbon fuels in the transportation field.

Recent research efforts have focused on the usage of hydrogen in homogeneous charge compression ignition (HCCI) engines, either as an engine fuel [11] or as an additive [12]. Experimental evidence suggests that hydrogen can be used as a primary fuel for HCCI engines, albeit in a very lean mixture ($0.1 < \Phi < 0.3$) due to its fast burning characteristics and high heat release rate. Advantages include lower NO_x emissions and higher efficiency than spark ignition (SI) for the range where it is possible to operate in HCCI mode. When it is used as an additive to hydrocarbon fuels, it was found that hydrogen stabilizes combustion in a natural gas HCCI engine under difficult operating conditions.

In the past few years, treatment of turbulence/chemistry interactions in HCCI engine simulations by probability density function (PDF) [13] has received considerable attention. Examples of PDF treatment of turbulence/chemistry interactions and of mixture stratification fall more or less into two broad categories.

The first category, which we shall call the *stochastic reactor* approach, includes methodologies in which the PDF is assumed to be spatially homogeneous and a zero-dimensional time evolution equation for the PDF is formulated to include the effects of piston movement, convective heat transfer to the walls, turbulent mixing, gas exchange, and possibly fuel injection. The closure of turbulent mixing is treated with conventional mixing models taken from turbulent combustion modeling [14]. However, one should note that the PDF equation is taken to be descriptive of the whole cylinder rather than of the local turbulent fluctuations, as is generally intended in turbulent combustion modeling [13]. Notable applications of the stochastic reactor approach will now be briefly summarized. A stochastic reactor model relying on a