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The effects of thermal and compositional stratification on the ignition and duration of homogeneous charge compression ignition combustion

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ABSTRACT

In this work, the effects of thermal and compositional stratification on the ignition and burn duration of homogeneous charge compression ignition (HCCI) combustion are studied with full-cycle 3D computational fluid dynamics (CFD) simulations with gasoline chemical kinetics performed during the closed portion of the cycle, from intake valve closing (IVC). The stratification was varied through the use of negative valve overlap (NVO) and positive valve overlap (PVO) breathing strategies. To remove charge energy and phasing effects from the simulation results, the fuel mass and ignition timing were held constant, while mean composition effects were isolated from those of local stratification by maintaining the same mean oxygen concentration, fuel–oxygen equivalence ratio and charge heat capacity. Fuel was premixed with the intake to avoid potential stratification effects arising from direct injection. With NVO, the incomplete mixing of the fresh charge with the large mass fraction of product gases retained within the cylinder from the previous combustion cycle leads to a 23% increase in the pre-ignition thermal stratification, and an order of magnitude increase in the levels of stratifications in fuel to oxygen equivalence ratio and oxygen mole fraction relative to the PVO strategy, which employs a premixed mixture of fresh and product gases. Under the conditions studied, the use of NVO resulted in a 30% increase in the 10–90% burn duration (CA10-90) compared to the PVO condition. Two additional analyses were performed to decouple the effects of thermal and compositional stratification. The first examined the reaction space (based on the ignition delay distribution within the charge prior to ignition) for both breathing strategies to quantify the inherent reactivity stratification. The second examined the more stratified NVO case with a quasi-dimensional multi-zone model. These analyses revealed that under the conditions studied, HCCI reactivity and combustion duration are governed primarily by thermal stratification and are largely insensitive to compositional stratification at the time of ignition.

1. Introduction

Homogeneous charge compression ignition (HCCI) is an advanced combustion mode for reciprocating internal combustion engines, which aims to achieve diesel-like efficiency while minimizing emissions of nitrogen oxides (NO_x) and soot [1–4]. HCCI requires higher unburned gas temperatures than conventional spark-ignited (SI) operation [5], since combustion is initiated through chemical kinetics rather than through spark discharge. To achieve the required temperature for auto-ignition, HCCI engines typically employ an increased compression ratio, along with a means for controlling the sensible internal energy of the charge at intake valve closing (IVC), either through the retention of hot residual combustion products, or through the external heating of the incoming charge (intake air heaters [6], bypassing the intercooler [7]), or through a combination of these methods.

One method to achieve HCCI is with conventional positive valve overlap (PVO), with premixed fuel, air and exhaust gas recirculation (EGR) [3,6]. This method has minimal compositional stratification within the charge owing to premixed operation [8]. Here, the intake air is typically heated to provide the thermal energy needed to achieve auto-ignition. Another method, appropriate for the control of auto-ignition phasing, is negative valve overlap (NVO) [9–14], where the exhaust valve is closed prematurely during the exhaust stroke in order to retain a large fraction of high

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temperature residual combustion products within the cylinder, which is then mixed with the cooler incoming fresh charge. To advance ignition timing, the charge temperature at IVC is increased by retaining higher levels of residual mass fraction through earlier closure of the exhaust valve. This strategy is particularly effective in managing hot internally recirculated exhaust gas (iEGR) on a cyclic basis, making NVO operation attractive for transient operation.

During NVO operation, hot residual gases and cooler fresh fuel–air mixture are mixed during the ignition delay period. If the mixing timescales are longer than the ignition delay, the combustion process will occur within a thermally and compositionally stratified charge, which could affect the local combustion regime. A series of direct numerical simulation (DNS) studies investigating this question have shown that combustion under HCCI conditions is chemically controlled [15–18]. In particular, Chen et al. [17] found that under typical HCCI engine conditions without significant stratification, unlike diesel combustion with direct injection, a reasonable approximation is that different locations in the cylinder interact only through pressure-work, with molecular mixing effects not having a large impact. The work of Bansal and Im investigating thermal and compositional stratification effects arrived at a similar conclusion [19]. Spontaneous wave-like ignition front propagation (sequential auto-ignition) [20] was observed for a case with pure thermal stratification and also for a case with uncorrelated thermal and equivalence ratio stratification, whereas near constant-volume combustion was observed for a case with negatively correlated thermal and equivalence ratio stratification. Finally, it was observed in one dimensional premixed flame modeling that burned gas temperatures on the order of 1400–1500 K are required to support premixed flames under HCCI conditions [21,22]. Achieving such temperatures would require relatively high levels of end-gas reaction progress during HCCI, with steep compositional and thermal gradients. Although flames can be supported under these conditions, the combustion mode within the compositional and thermal gradient of the flame transitions from deflagration to the spontaneous ignition front regime at end-gas thermal runaway [23]; the end-gas mass consumed by the front during the auto-ignition process was also minimal [23]. These results suggest that the chemically controlled combustion assumption employed in HCCI combustion modeling is appropriate for the modeling of this combustion process [24–31]. It must be noted that the CFD combustion model used in the current work also treats every cell as a homogeneous reactor, as in [24–31], and thus does not account for turbulence–chemistry interactions (TCI). Further, the Reynolds Averaged Navier–Stokes (RANS) approach used in this work does not capture turbulent fluctuations in the temperature and equivalence ratio fields. However, as it is shown later in this document, adopting the RANS well-mixed approach for HCCI combustion produces good results compared to experiments even for NVO cases with higher stratification, in terms of global pressure profiles and burn rates, which are the focus of this study. A more sophisticated combustion model that also accounts for TCI in conjunction with large eddy simulation (LES) could be adopted in future work.

Other researchers have experimentally investigated the implications of NVO on charge stratification and HCCI combustion. In their pioneering optical engine work, Rothamer et al. [8] compare the stratification during NVO against PVO operation with little valve overlap. They found significant thermal and compositional stratification within the charge prior to ignition with NVO and speculated that the enhanced stratification could extend the burn duration. However, they do not say what the relative importance of thermal versus compositional stratification is with respect to burn duration. Babajimopoulos et al. [28] numerically investigated the effect of accounting for both thermal and compositional stratification within computational fluid dynamics (CFD) simulations of HCCI combustion and came to the conclusion that under the conditions studied by them, neglecting compositional stratification does not affect prediction of ignition timing significantly. However, unlike the current work, their study did not examine burn rates, and did not attempt to correlate the effect of stratification to sequential autoignition and burn duration. Joelsson et al. [32] performed large eddy simulations (LES) to determine distributions resulting from NVO operation followed by multi-zone kinetics calculations. They found that under higher NVO conditions a zone with a preferred mixture composition and temperature ignited first. More recently, Olesky et al. [14] studied the effect of NVO operation on HCCI combustion duration by trading off intake air heating with NVO duration over a range of combustion phasings. They found that for a given combustion phasing, increasing the level of NVO consistently increased the 10–90% burn duration compared to operation with less NVO and elevated intake temperature. They hypothesized that the observed increase in burn duration was due to a combination of effects such as lower oxygen concentration (a chemical kinetic effect) and higher mixture specific heat (a thermodynamic effect) resulting from replacing some of the air in the charge with residual as NVO increased. They also proposed that additional thermal stratification could be generated from the higher levels of NVO, which in turn would increase the burn duration.

Olesky et al. also examined the influence of NVO, and its potential thermal and compositional stratification, on spark assisted compression ignition (SACI) combustion at constant spark timing and fueling [33]. They varied internal residual through a relatively small (26° crank angle) adjustment in NVO. External EGR (eEGR) was adjusted in conjunction with intake air preheating to maintain constant the total residual fraction and inferred temperature at intake valve closing. The resulting variations in NVO had little to no effect on combustion, implying that the relative variations in thermal and compositional stratification associated with NVO were minor under these conditions. Considering the narrow range of NVO used in this study, it cannot be concluded that such effects are not important when evaluated over a much broader range of valve events.

There is presently an understanding gap in the importance of thermal and compositional stratification to the overall reactivity stratification controlling the ignition and duration of HCCI combustion under engine relevant conditions. While previous experiments have shown that stratification does indeed vary with breathing strategy [14] and also how such variations may affect HCCI combustion duration [8], mean compositional effects, such as oxygen concentration and heat capacity, are interwoven with local stratification effects in these studies. Therefore, the objective of the current work is to evaluate stratification effects, in isolation from mean composition effects, on the charge reactivity distribution and the consequent effect of this distribution on HCCI ignition conditions and combustion duration.

To this end, full-cycle CFD KIVA-3V [34] simulations are performed with fully-coupled multi-zone gasoline chemical kinetics for PVO with external EGR dilution (eEGR) and for NVO with internal exhaust gas recirculation (iEGR). Potential factors complicating the analysis, such as the localized evaporative cooling and stratification associated with direct injection [35–41] are avoided through the use of a premixed fuel–air mixture at the intake for the NVO condition and a premixed fuel–air–eEGR mixture at the intake for the PVO condition. Both NVO and PVO cases were configured to have the same mean composition in terms of oxygen concentration and heat capacity (C_p), fueling and overall level of charge dilution at intake valve closing (IVC) through the respective manipulation of internal (iEGR) and external (eEGR) recirculated exhaust gas. Additional intake charge heating is used for the