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Computational study of the pressure dependence of sequential auto-ignition for partial fuel stratification with gasoline

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Abstract

Fuel stratification is a potential strategy for reducing the maximum pressure rise rate in HCCI engines. Simulations of Partial Fuel Stratification (PFS) have been performed using CONVERGE with a 96-species reduced mechanism for a 4-component gasoline surrogate. Comparison is made to experimental data from the Sandia HCCI engine at a compression ratio 14:1 at intake pressures of 1 bar and 2 bar. Analysis of the heat release and temperature in the different equivalence ratio (φ) regions reveals that sequential auto-ignition of the stratified charge occurs in order of increasing φ for 1 bar intake pressure but in order of decreasing φ for 2 bar intake pressure. Increased low- and intermediate-temperature heat release at 2 bar intake pressure compensates for decreased temperatures in higher-φ regions due to evaporative cooling from the liquid fuel spray and decreased compression heating from lower values of the ratio of specific heats. At 1 bar intake pressure, the premixed portion of the charge auto-ignites before the highest-φ regions and the sequential auto-ignition occurs too fast for useful reduction of the maximum pressure rise rate compared to HCCI. Conversely, at 2 bar intake pressure, the premixed portion of the charge auto-ignites last, after the higher-φ regions. More importantly, the sequential auto-ignition occurs over a longer time period than at 1 bar intake pressure such that a sizable reduction in the maximum pressure rise rate compared to HCCI can be achieved.

Keywords: Gasoline; Reduced; Mechanism; Stratification; Auto-ignition

1. Introduction

In order to limit carbon dioxide and pollutant emissions from internal combustion (IC) engines, next-generation low-temperature compression ignition (CI) combustion modes that reduce exhaust emissions and improve thermal efficiency are currently being explored. Homogeneous Charge Compression Ignition (HCCI) is an advanced low-temperature combustion (LTC) mode that has received substantial research attention. For HCCI at high loads, however, extremely rapid combustion can occur leading to knock

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(pressure oscillations) and, ultimately, engine damage. Lean fuel-air mixtures or high levels of exhaust gas recirculation (EGR) are required to lower the heat release rate (*HRR*) such that the maximum pressure rise rate (PRR_{max}) is acceptable [1]. Although homogeneous fuel mixtures are targeted in HCCI combustion, thermal stratification has been shown to play an important role in dictating *HRR* and PRR_{max} [2–4]. Fuel stratification has also been shown to influence *HRR* and PRR_{max} [5–9].

Partial Fuel Stratification (PFS) aims to reduce PRR_{max} by using fuel stratification to prolong combustion [5–9] and enable engine operation at high load conditions. PFS is accomplished by mixing the majority of the fuel with intake air and direct-injecting (DI) the rest during the compression stroke. The goal of preparing a stratified mixture is to promote sequential auto-ignition that reduces PRR_{max}. The fuel auto-ignition chemistry is critical for PFS and the behavior of PFS depends on how the auto-ignition characteristics of the fuel (or fuel-blend) change with equivalence ratio (φ) and if the fuel exhibits single- or multi-stage ignition [6].

The φ-sensitivity of a fuel describes how its auto-ignition characteristics change with φ and is an indicator of how a fuel will respond to stratification [5–7]. A fuel is considered φ-sensitive if changing φ results in a large change in HCCI combustion phasing. For gasoline at ambient intake pressure, increasing φ delays the hot-ignition (thermal-runaway) timing because the reduced ratio of specific heats ($\gamma = c_p/c_v$) decreases the compressed-gas temperature. Thus, gasoline is not φ-sensitive at ambient intake pressure. Interestingly, gasoline becomes φ-sensitive at boosted intake pressure because the pre-ignition reactions become more active at increased pressure and are more prominent for larger φ. PFS is expected to result in multi-stage ignition for φ-sensitive fuels where the heat released from pre-ignition reactions increases with φ.

In a review of CI engines [2], Dec notes that CI engine modeling requires improved chemical-kinetic models that accurately predict low temperature heat release (LTHR), intermediate temperature heat release (ITHR), pressure-boost effects, and the behavior of realistic fuels. Accurate prediction of LTHR is important because LTHR influences the chemistry leading up to hot ignition [10]. Additionally, the higher temperature rise rate prior to hot ignition resulting from LTHR reduces the influence of random fluctuations in the charge temperature on the hot ignition timing [11]. Prediction of ITHR is important because ITHR can cause the in-cylinder temperature to continue to increase during piston expansion after top dead center (TDC) before hot-ignition [12]. Accurately predicting the effects of pressure-boost is important because the LTHR/ITHR characteristics of a fuel can change with pressure (e.g. gasoline).

The current work uses CONVERGE [13], a commercial computational fluid dynamics (CFD) and chemical kinetics code, to computationally investigate PFS for two representative cases from [5] at intake pressures of $P_{in} = 1$ bar and $P_{in} = 2$ bar using a 96-species reduced mechanism [14] for a 4-component gasoline surrogate. The objective of this work is to perform detailed analysis of the heat release and temperature in the different φ regions to elucidate how the interplay between pre-ignition reactions, evaporative cooling, and specific heat ratio effects changes with intake pressure for gasoline.

2. CONVERGE

Simulations of PFS were performed using CONVERGE, which employs a cut-cell Cartesian method for grid generation, for the Sandia HCCI engine [5] with a grid spacing of 2 mm. A schematic of the computational grid is shown in Fig. 1 and engine specifications are listed in Table 1 (values in parentheses indicate experimental values that differ from the associated value used in the simulation). The geometric compression ratio (CR) of the computational mesh is 13.65:1, which is slightly lower than the 14:1 used in the experiment in order to match the motored pressure trace. The head gasket crevice is included in the computational mesh and a piston ring crevice model is used rather than direct meshing of the piston ring crevices. Simulations are run from 360°BTDC to 90°ATDC. Due to the computational cost, a grid resolution study was not performed with finer grids; however, coarsening the grid resolution to 4 mm tended to advance combustion phasing by ~2°CA.

Gasoline is modeled by a 4-component surrogate comprised of 57% iso-octane (iC_8H_{18}), 16% n-heptane (nC_7H_{16}), 23% toluene ($C_6H_5CH_3$), and 4% 2-pentene (C_5H_{10}-2) [15]. The chemistry

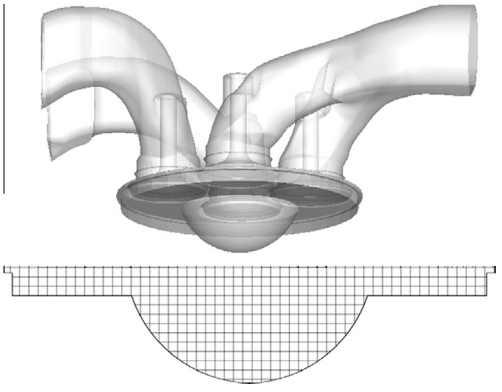

Fig. 1. Computational mesh of Sandia HCCI engine at TDC with a grid spacing of 2 mm.

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