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Ignition of a lean PRF/air mixture under RCCI/SCCI conditions: Chemical aspects

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Abstract

Chemical aspects of the ignition of a primary reference fuel (PRF)/air mixture under reactivity controlled compression ignition (RCCI) and stratified charge compression ignition (SCCI) conditions are investigated by analyzing two-dimensional direct numerical simulation (DNS) data with chemical explosive mode (CEM) analysis. CEMA is adopted to provide fundamental insights into the ignition process by identifying controlling species and elementary reactions at different locations and times. It is found that at the first ignition delay, low-temperature chemistry (LTC) represented by the isomerization of alkylperoxy radical, chain branching reactions of keto-hydroperoxide, and H-atom abstraction of *n*-heptane is predominant for both RCCI and SCCI combustion. In addition, explosion index and participation index analyses together with conditional means on temperature verify that low-temperature heat release (LTHR) from local mixtures with relatively-high *n*-heptane concentration occurs more intensively in RCCI combustion than in SCCI combustion, which ultimately advances the overall RCCI combustion and distributes its heat release rate over time. It is also found that at the onset of the main combustion, high-temperature heat release (HTHR) occurs primarily in thin deflagrations where temperature, CO, and OH are found to be the most important species for the combustion. The conversion reaction of CO to CO_2 and hydrogen chemistry are identified as important reactions for HTHR. The overall RCCI/SCCI combustion can be understood by mapping the variation of 2-D RCCI/SCCI combustion in temperature space onto the temporal evolution of 0-D ignition.

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1. Introduction

Homogeneous-charge compression ignition (HCCI) engines have been developed because they can provide high thermal efficiency and ultra-low emissions compared to the conventional IC engines. However, the development of prototype HCCI engine has been prohibited by its narrow operating range and difficulties in combustion-phasing control. To overcome these problems, some variants of HCCI engines including reactivity controlled compression ignition (RCCI) and stratified charge compression ignition (SCCI) have been proposed thus far. To introduce in-cylinder fuel stratification, dual-fuel RCCI combustion uses in-cylinder blend of two fuels with different ignition characteristics: low reactivity fuel (e.g., *iso*-octane) supplied through port-fuel injection (PFI) and directly-injected high reactivity fuel (e.g., *n*-heptane). However, SCCI combustion uses only a single fuel with the same two-stage injection strategy. With optimized blending of two fuels rather than a single fuel, RCCI combustion can provide better combustion-phasing control with lower pressure-rise rate (PRR) [1,2].

There have been numerous experimental and computational studies of HCCI-type engines, which primarily focus on the bulk engine characteristics such as emissions and operating performances [1–10]. However, only a few studies on the chemical combustion process of RCCI/SCCI combustion have been performed [3,9,11–15]. For instance, Kokjohn et al. [3] numerically investigated the combustion characteristics of E85-diesel RCCI combustion and found that formaldehyde (CH_2O) and hydroxyl (OH) radicals are the key species for the first- and second-stage ignitions, respectively, and the less reactive fuel was consumed nearly simultaneously with formaldehyde.

From the spectroscopic and chemical-kinetic analysis of HCCI combustion, Hwang et al. [12] identified that significant amount of low-temperature heat release (LTHR) of PRF80/air mixtures occurs in the range of 760 to 880 K with significant formaldehyde production, resulting in rapid temperature rise during the intermediate-temperature heat release (ITHR) and thereby advancing the main combustion. Westbrook [11] pointed out that the overall HCCI combustion can be advanced by adopting variations in engine parameters such as pressure, temperature, and equivalence ratio which enable in-cylinder fuel/air mixtures to reach the H_2O_2 decomposition temperature at earlier time.

Recently, Vuilleumier et al. [15] found from an experimental and modeling study that the addition of highly reactive *n*-heptane content induces the increase of ITHR, eventually triggering high-temperature heat release (HTHR) with a significant formaldehyde accumulation. In addition, they identified the dominant reaction pathways: H-atom abstraction from *n*-heptane by OH and the addition of heptyl radicals to O_2. These previous studies, however, were either RANS and low-dimensional analyses or optical measurement with high uncertainty to discern individual fuel species such that further understanding of the chemical aspects of RCCI/SCCI combustion is still needed.

More recently, Luong et al. [9] investigated the ignition characteristics of *n*-heptane/air mixture under HCCI/SCCI conditions by performing 2-D direct numerical simulations (DNSs). They identified important species and reactions for HCC/SCCI combustion by using chemical explosive mode analysis (CEMA). However, CEMA has not been applied to RCCI combustion. Therefore, the objective of the present study is to provide insights into the chemical ignition process of PRF/air mixture under RCCI/SCCI conditions by analyzing 2-D DNS data with CEMA.

For this purpose, we use the data set generated from 2-D DNSs of the ignition of a lean PRF/air mixture under RCCI/SCCI conditions by Luong et al. [16]. From this study, it is found that the overall combustion of RCCI is more advanced and more distributed in time than that of SCCI due to the dominant role of reactivity stratification in inducing more deflagration mode of combustion in the low-to-intermediate temperature regime. However, both RCCI and SCCI have similar overall combustion characteristics in the high-temperature regime because the ignition of the PRF/air mixture becomes less sensitive to reactivity stratification and/or equivalence ratio.

2. Methodology

To investigate the chemical aspects of RCCI and SCCI combustion, we analyze 2-D DNS data set in [16] using CEMA. The 2-D DNSs of the ignition of the PRF/air mixture under RCCI and SCCI conditions were simulated using the Sandia compressible DNS code [17], S3D, with a

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