# RCCI/SCCI 조건하에서 희박 PRF/공기 혼합물의 점화에 관한 직접수치모사를 이용한 비교 연구

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# DNSs of the Ignition of a Lean PRF/Air Mixture under RCCI/SCCI Conditions: A Comparative Study

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## ABSTRACT

A comparative DNS study of the ignition characteristics of dual-fueled reactivity controlled compression ignition (RCCI) and stratification charge compression ignition (SCCI) is investigated using a 116-species reduced primary reference fuel (PRF) mechanism. In the RCCI combustion, two PRF fuels (*n*-heptane and *iso*-octane) with opposite autoignition characteristics are separatedly supplied and in-cylinder blended such that spatial variations in fuel reactivity, fuel concentration and temperature are achieved. In the SCCI combustion, however, just a single fuel (PRF50) is used such that only fuel concentration and temperature inhomoginieties are obtained. Because three factors, rather than only two as in SCCI combustion, govern the overall RCCI combustion, combustion timing and combustion duration or heat release rate of RCCI combustion are flexibly and effectively controlled. It is found that the overall RCCI combustion occurs much earlier and its combustion duration is longer compared to SCC combustionI. Moreover, the negative temperature coefficient (NTC) has a positive effect on enhancing RCCI combustion by inducing a shorter combustion timing and a longer combustion duration as a result of the occurrence of a predominant low-speed deflagration-combustion mode.

Key Words: DNS, HCCI, RCCI, SCCI, PRF reduced mechanism, mixture inhomogeneities

Reactivity controlled compression ignition (RCCI) and stratified-charge compression ignition (SCCI), promising variants of homogeneous charge compression ignition (HCCI), have received considerable attention from the engine community because of their better combustion-phasing and HRR control, lower fuel consumption and emissions. Unlike SCCI using a single fuel, RCCI uses two different fuels with opposite ignition characteristics: one fuel with low-reactivity and the other with high-reactivity [1].

For both RCCI and SCCI concepts, appropriate stratified mixture allows a longer combustion duration by a sequential combustion ignition, resulting in a smoother combustion process under high-load conditions. The underlying combustion process is switching the combustion mode from a high-speed spontaneous auto-ignition mode into a wave-like low-speed deflagrative mode [2-7].

Different levels of in-cylinder stratified fuel/air mixtures can be intensionally achieved by (i) varying the mass fraction of port-fuel injection (PFI), $m_1$, and direct-fuel injection (DFI), $m_2$, and (ii) adjusting the injection timing. Generally, PFI is used to create nearly homogeneous fuel/air mixture; while, DFI is used to introduce some levels of in-cylinder mixture inhomogeneities close to the top dead center (TDC) prior to the combustion event. With an appropriate fuel preparation strategy, spatially optimal variations in fuel reactivity, fuel concentration and temperature of RCCI are straightforwardly created by using two different fuels of low- and high-reactivity; whereas, under SCCI conditions, only fuel concentration and temperature inhomogeneities are achieved because a single fuel is used. As such, RCCI probably provides more easy

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controllability over the combustion process: flexibly tailoring ignition timing and combustion duration, thereby effectively preventing a rapid pressure rise rate (PRR) and significantly extending a limited HCCI operating range to a higher load.

Numerous experimental and computational studies on SCCI combustion have been conducted [1-7]. Using 2-D DNSs, Yoo et al. [2] and Luong et al. [6] revealed that ignition characteristics of two-stage ignition fuels can be significantly changed with (i) different mean temperatures, $T_0$, in the NTC region and (ii) different levels of $T'$ and $\phi'$. Luong et al. [6] also found that $T_0$ lying in the NTC regime together with a negative $T-\phi$ distribution has a positive effect on advancing the overall ignition and prolonging combustion duration, and thus spreading out HRR and PRR [6]. It is believed that $T_0$ lying in the NTC regime also has a positive effect on enhancing the overall RCCI combustion process. However, up to now, there are no DNS studies on RCCI combustion and a fundamental understanding of the influence $T_0$ within the NTC regime on RCCI ignition is still elusive.

The objective of the present study, therefore, is to provide a fundamental comparison of the ignition characteristic and combustion mode between RCCI and SCCI with $T_0$ lying in the NTC regime by using 2-D DNSs. The 1-D and 2-D DNSs are sequentially performed by varying two key parameters: (1) $r'$ where $r' \equiv m_2'/m_2$ and (2) $T'$. In this study, a 116-species reduced PRF mechanism is adopted in which *n*-heptane and *iso*-octane are respectively representative of high- and low-reactivity fuels. Details of the PRF reduced mechanism can be found in [4].

The Sandia DNS code, S3D, was used to simulate RCCI and SCCI combustion process. The computational domain is a 2-D square box with each size, $L$, of 3.2 mm, discretized with a grid size of 2.5 $\mu m$. For consistent comparison, mean equivalence ratio, $\phi_0 = 0.45$, an initial uniform pressure, $p_0 = 40$ atm, and $T_0 =$ 900 K are initially specified for all DNSs. Similarly, PRF50 (*iso*-octane/*n*-heptane mixture fraction by volume) is chosen as a fuel for both RCCI and SCCI configurations. Particularly, in RCCI cases, $m_1$ and $m_2$ are *iso*-octane and *n*-heptane respectively and their corresponding mean PRF number is PRF50; while, in SCCI cases, both $m_1$ and $m_2$ are PRF50. In reality, $m_1$ and the entire air are homogeneously premixed; while, $m_2$ is directly introduced and mixed in cylinder with $m_1$ to generate some degrees of mixture stratification. Similar concepts are applied in the present study.

For comparison, $r' \equiv m_2'/m_2$, is used for both RCCI and SCCI configurations to initialize different levels mixture stratification. After the initialization using $r'$, the local PRF number, equivalence ratio can be easily calculated from the local mass fractions of *n*-heptane, *iso*-octane and air as representatively shown in Fig. 1. From the overall PRF and $\phi$ distribution, the corresponding mean and root mean square (RMS) value of fuel reactivity and equivalence ratio also can be calculated. Here $r' =$ 0.22 or 0.44 are intentionally selected such that $\phi$ lies in the optimal region to maintain low-temperature combustion and nearly no engine-out emissions. At $r' =$ 0.44, for instance, $\phi$ for both RCCI and SCCI cases varies approximately from 0.85 to 0.25, which lies in the optimal range for RCCI/SCCI combustion. Moreover, the corresponding calculated $PRF'$ and $\phi'$ are 12.8 and 0.1 respectively under RCCI conditions; and are 0.0 and 0.1 respectively under SCCI conditions.

Due to latent heat from fuel vaporization of the late second direct injection, either a $PRF-\phi$ field for RCCI or a $T-\phi$ field for SCCI prior to the combustion event were experimentally found to be negatively-

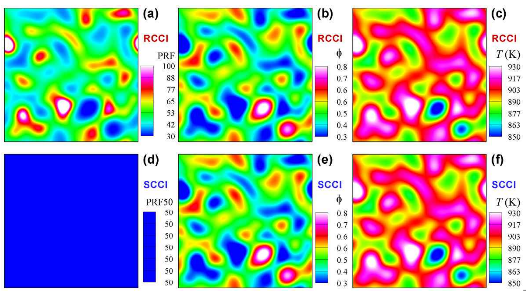


**Fig. 1** Initial PRF, $\phi$ and $T$ fields under (a-c) RCCI and (d-f) SCCI configuration at $r' =$ 0.44 and $T' = 15$ K.

| Type | $T_0$ (K) | $T'$ (K) | $PRF_0$ | $PRF'$ | $\tau_{ig}^0$ (ms) |
|---|---|---|---|---|---|
| RCCI | 900 | 0 | PRF50 | 0.44 | 2.2 |
| RCCI | 900 | 15 | PRF50 | 0.44 | 2.2 |
| SCCI | 900 | 0 | PRF50 | 0 | 2.2 |
| SCCI | 900 | 15 | PRF50 | 0 | 2.2 |

**Table 1** Physical parameters of the 2-D DNS

correlated (NC) and $T'$ is about 15−25 K. Hence, in the present study, NC fields of $PRF-\phi$ and $T-\phi$ distribution are respectively specified for RCCI and SCCI configurations as representatively shown in Fig. 1, and $T'=15$ and 30 K are chosen.

In short, three factors including (i) fuel reactivity, (ii) equivalence ratio, and (iii) temperature variations are initially generated to control RCCI combustion process; while, for SCCI, only two factors: (i) equivalence ratio, and (ii) temperature variations coexist and control SCCI combustion process.

The homogeneous ignition delay, $\tau_{ig}^0$, of PRF50 at $T_0$ = 900 K, $\phi_0$ = 0.45 and $p_0$ = 40 atm is approximately 2.2 ms, where $T_0$ = 900 K lies within the NTC regime. The turbulence intensity, $u'$ = 0.5 m/s, length scale, $l_e$ = 1.0 mm are specified for all DNS cases. The corresponding turbulence time scale, $\tau_t$, is 2.0 m/s, which is comparable to $\tau_{ig}^0$. The most energetic length scale of the temperature fluctuation, $l_{Te}$ is 1.0 mm. The detailed intial parameters of 2-D DNSs are given in Table 1.

Based on 0-D ignition delays of different PRFs and $\phi$ as a function of temperature, the ignition delay range of RCCI and SCCI can roughly be estimated as shown in Fig. 2. As readily seen in Fig. 2, the ignition range and the shortest $\tau_{ig}^0$ of RCCI respectively are much wider and significantly smaller than that of SCCI. Therefore, it can be expected that under the same initial conditions, the combustion duration and the start of combustion for RCCI cases occur longer and sooner compared to those of SCCI cases.

In the first 1-D parametric study, the temporal evolutions of mean HRR, $\bar{\dot{q}}$, with different $r'$ and $T'$ are shown in Fig. 4. As expected, (i) the onset of combustion of RCCI cases occurs much earlier and its combustion duration is wider compared to the corresponding SCCI cases; (ii) $\tau_{ig}$ is advanced more with increasing $T'$ due to $T_0$ lying in the NTC regime. Additionally, with increasing $r'$, the NTC regime shows a stronger effect on advancing $\tau_{ig}$ for RCCI cases (see the cases with $r'$ = 0.44 and $T'$ = 0 K and 30 K in Fig. 3). On the contrary, with only thermal stratification ($r'$ = 0), $\tau_{ig}$ remain nearly the

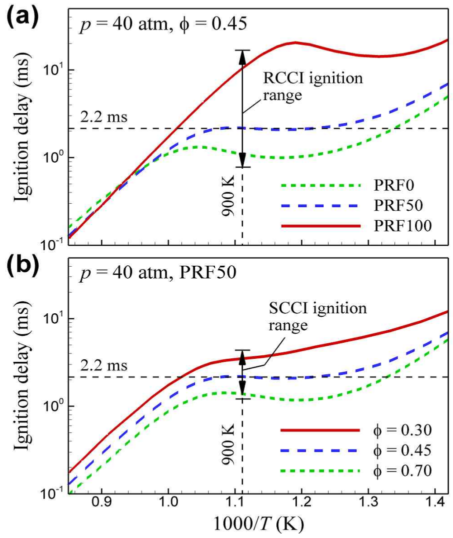


**Fig. 2** 0-D ignition delays at a constant volume, $\phi_0$ = 0.45, and $p_0$ = 40 atm as a function of initial temperature for (a) different PRFs and (b) different $\phi$.

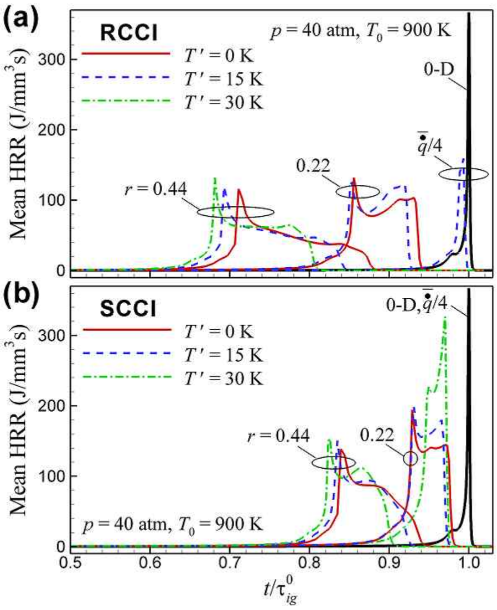


Fig. 3 Temporal evolution of HRR for 1-D DNSs of (a) RCCI, and (b) SCCI. The black line represent the 0-D homogeneous ignition.

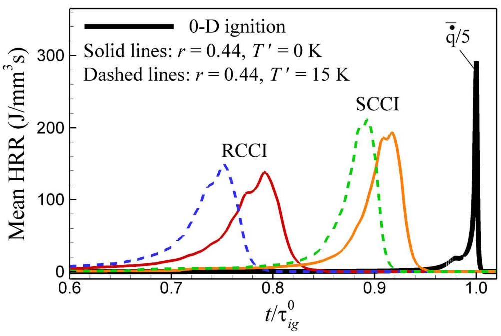


Fig. 4 Temporal evolution of HRR for 2-D DNSs of RCCI and SCCI.

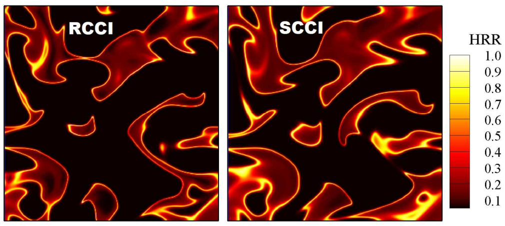


Fig. 5 Contours of HRR at $\tau_{ig}$ under RCCI and SCCI conditions ($r'=0.44$ and $T'=15\,\mathrm{K}$).

same 0-D ignition, $\tau_{ig}^{0}$. Because of a longer combustion duration in RCCI cases, $\bar{\dot{q}}$ is more distributed over time and the peak $\bar{\dot{q}}$ is much lower than those of the corresponding SCCI cases.

A similar behavior is observed in the second 2-D parametric study as shown in Fig. 4, except a slight change in $\tau_{ig}$. $\tau_{ig}$ is advanced further because of the effect of the NTC regime.

Figure. 5 shows that RCCI combustion occurs in thinner reaction sheets and a relatively lower HRR, qualitatively verifying that combustion process of RCCI induces more wave-like deflagrations than that of SCCI. As such, the combustion duration is elongated.

A comparative DNS study of RCCI and SCCI combustion with $T_0$ lying the NTC regime was conducted using a 116-species reduced PRF mechanism. The RCCI concept use two different reactivity fuels (*iso*-octane is less reactive and *n*-heptane is highly reactive); while the SCCI concept use a single fuel with a two-stage ignition fuel, PRF50. It is found that compared to the same SCCI case (i) the overall RCCI combustion is greatly advanced and its combustion process occurs longer, resulting a more distributed HRR and significantly lower peak HRR; (ii) $\tau_{ig}$ is increased more for both RCCI and SCCI cases when $T_0$ lies in the NTC regime, however, the NTC regime has a more influence on advancing RCCI combustion (a shorter $\tau_{ig}$); (iii) RCCI produces more low-speed wave-like deflagrations than SCCI, which in turn prolongs the combustion duration as such HRR or PRR are significantly reduced.

These results suggest the RCCI concept is better than the SCCI concept in manipulating the overall combustion; it is more flexible in adjusting ignition timing, controlling the rate of heat release, and promisingly extending to a higher load.

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