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

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1 Introduction

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

Both RCCI and SCCI use in-cylinder mixture stratification to generate a sequential combustion ignition, resulting in a smoother combustion process under high-load conditions. The underlying combustion process is to switch the combustion mode from a high-speed spontaneous auto-ignition into a wave-like low-speed deflagration and as such, a longer combustion duration is obtained [1].

Different levels of in-cylinder mixture stratification can be intentionally achieved by (1) varying the mass fraction of port-fuel injection (PFI), m_1, and direct-fuel injection (DFI), m_2, and by (2) adjusting the injection timing. Generally, m_1 is used to generate a nearly homogeneous fuel/air mixture, while m_2 is used to introduce some levels of in-cylinder fuel stratification close to the top dead center (TDC) prior to the combustion event. For RCCI, m_1 and m_2 are two different fuels of low and high reactivity, while being the same fuel for SCCI. Because of using two fuels with different reactivity, spatial variations in fuel reactivity, fuel concentration and temperature are generated for RCCI; whereas, only fuel concentration and temperature inhomogeneities are generated in the cylinder for SCCI. As such, compared with SCCI, RCCI may provide easier controllability over the combustion process: flexibly-tailoring ignition timing and combustion duration, thereby effectively preventing an excessive 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 [1-6]. Using 2-D DNSs, Luong et al. [6] revealed that ignition characteristics of SCCI can be significantly changed with (1) different mean temperatures, T_0, within/near the negative temperature coefficient (NTC) regime and (2) different levels of T' and ϕ'. They also found T_0 lying in the NTC regime together with a negative T–ϕ distribution has a positive effect on advancing the overall ignition and prolonging combustion duration, and thus significantly spreading out HRR and PRR. The RCCI combustion process of RCCI may also be changed with different T_0 lying within/near the NTC regime. However, up to now there is no DNS study on RCCI combustion, and a fundamental understanding of the influence T_0 within/outside the NTC regime on RCCI ignition is still unconclusive.

The objective of the present study, therefore, is to provide a better understanding of the effects of different T_0 within/near and outside the NTC regime on the ignition characteristic of RCCI; and a comparison of RCCI and SCCI combustion is also investigated by using 2-D DNSs. 2-D DNSs are performed by varying two key parameters: (1) mean temperature, and (2) temperature fluctuation. In this study, a 116-species reduced primary reference fuel (PRF) mechanism is adopted in which *n*-heptane and *iso*-octane are respectively representative of high- and low-reactivity fuels. Note that PRF

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has been widely used as a viable surrogate for practical engine fuels and details of the PRF reduced mechanism can be found in [4].

2 Numerical method and initial conditions

The Sandia DNS code, S3D, was used to simulate RCCI/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 μm. For all DNSs, mean equivalence ratio, $\phi_0 = 0.45$, an initial uniform pressure, $p_0 = 40$ atm are initially specified. Global reactivity for RCCI is PRF50, which is also the fuel used for SCCI. Particularly, for RCCI cases, m_1 and m_2 are *iso*-octane and *n*-heptane, respectively, to represent low- and high-reactivity fuel. The corresponding PRF number of the mixture, m_1+m_2, is PRF50; while for SCCI cases, both m_1 and m_2 are PRF50. In reality, m_1 and intake air are homogeneously premixed; while, m_2 is directly introduced and mixed in the cylinder to generate a certain degree of mixture stratification as conceptually shown in Fig. 1. Similar concepts are applied in the present study.

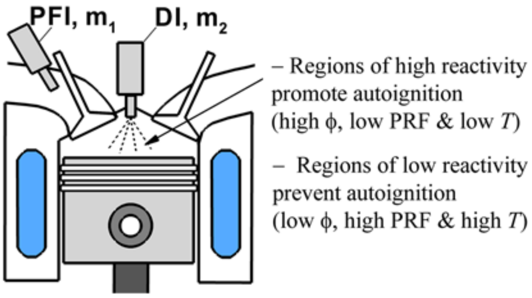

Figure 1. RCCI operating concept. m_1 and m_2 are the mass fraction of low- and high-reactivity fuel, respectively. PFI and DI denote port fuel injection and direct injection, respectively.

For consistent comparison, r defined as $r \equiv m_2'/ m_2$ is used to describe degrees of mixture stratification for both RCCI/SCCI configurations. After the initialization using r, local PRF number and equivalence ratio, and their corresponding mean and root mean square (RMS) value can be easily calculated from the local mass fractions of *n*-heptane, *iso*-octane and air. Here $r = 0.44$ is intentionally selected such that ϕ lies in the optimal range of RCCI/SCCI combustion ($0.25 < \phi < 0.85$) to maintain low-temperature combustion and nearly no engine-out emissions. With $r = 0.44$, the corresponding calculated PRF'–ϕ' for RCCI and SCC are 12.8–0.1 and 0.0–0.1, respectively.

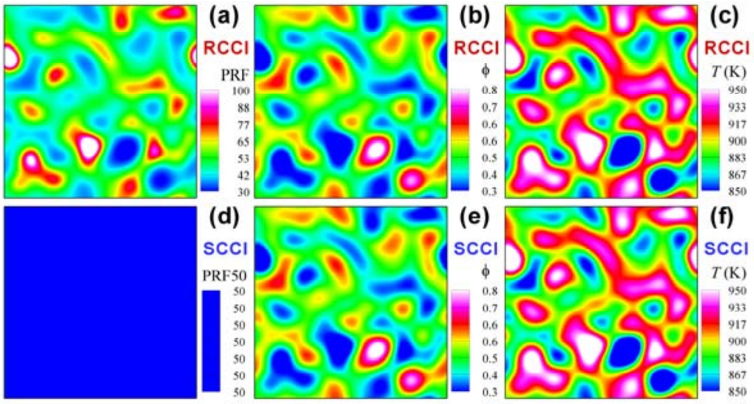

Figure 2. Initial PRF, equivalence ratio, and temperature fields of (a–c) RCCI and (d–f) SCCI configuration for Case 5 and Case 8, respectively.

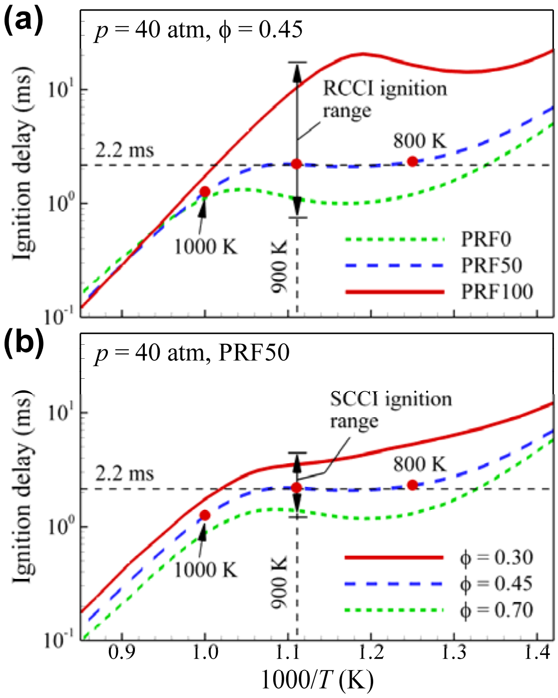

Figure 3. 0-D ignition delays of PRF/air mixtures as a function of initial temperature for (a) different PRFs and (b) different ϕ at $p_0 = 40$ atm.

Due to the evaporative cooling of the second late-direct injection together with a short mixing time, negatively-correlated (NC) T–ϕ distributions can exist prior to the combustion event. This is also demonstrated by an experimental study of SCCI, and T' was found about 15–30 K. In the present DNS study, T' of 15 and 30 K are therefore chosen, and NC T–ϕ distribution fields are also specified for both RCCI/SCCI configurations as representatively shown in Fig. 2. As seen, three factors including (1) fuel reactivity, (2) equivalence ratio, and (3) temperature inhomogeneities are present; while, for SCCI only two factors: (1) equivalence ratio, and (2) temperature variations coexist.

Figure 3 shows 0-D ignition delays of PRF/air mixture as a function of initial temperature for different PRFs and ϕ, and the ignition delay ranges of RCCI and SCCI at T_2 are roughly estimated. As readily observed in Fig. 3, the shortest τ_{ig}^0 and the ignition range of RCCI within/near the NTC regime are much smaller and longer, respectively than those of SCCI. Therefore, it can be expected that under the same initial conditions, the onset of main combustion and combustion duration of RCCI cases occur earlier and longer compared to those of SCCI. However, the shortest τ_{ig}^0 and the ignition range of RCCI with T_0 outside the NTC regime are not much different with those of SCCI. Therefore, three initial mean temperatures, T_1, T_2 and T_3 of 800, 900 and 1000 K, respectively, are chosen to examine the effects of initial low-, intermediate-, and high-mean temperatures on the ignition characteristics of RCCI/SCCI. Under the condition of $p_0 = 40$ atm and $\phi_0 = 0.45$, the homogeneous ignition delays of PRF50/air mixture for T_1, T_2 and T_3 are approximately 2.30, 2.20 and 1.25 ms, respectively.

An isotropic kinetic energy spectrum function by Passot-Pouquet together with different random numbers is used to prescribe the initial fields of turbulence, temperature and concentration. The most energetic length scales of turbulence, temperature and fuel stratifications, l_e, l_{Te}, and l_{me} are 1.0 mm for all DNS cases. The turbulence intensities are carefully selected such that the corresponding turbulence time scale, τ_t is comparable to τ_{ig}^0 ($\tau_t/\tau_{ig}^0 \sim O(1)$) and hence, most effective turbulent mixing of initial mixtures can be elucidated in the present DNS study. The detailed initial parameters of 2-D DNSs are given in Table 1.

Table 1: Physical parameters of the DNS cases

Case	Type	T_0	T'	PRF	PRF′	ϕ_0	ϕ'	l_e	l_{Te}	l_{me}	u'	τ_t	τ_{ig}^0
		(K)	(K)					(mm)	(mm)	(mm)	(m/s)	(ms)	(ms)
1	RCCI	800	30	50	12.8	0.45	0.1	1.0	1.0	1.0	0.5	2.0	2.30
2	SCCI	800	30	50	-	0.45	0.1	1.0	1.0	1.0	0.5	2.0	2.30
3	RCCI	900	0	50	12.8	0.45	0.1	1.0	1.0	1.0	0.5	2.0	2.20
4	RCCI	900	15	50	12.8	0.45	0.1	1.0	1.0	1.0	0.5	2.0	2.20
5	RCCI	900	30	50	12.8	0.45	0.1	1.0	1.0	1.0	0.5	2.0	2.20
6	SCCI	900	0	50	-	0.45	0.1	1.0	1.0	1.0	0.5	2.0	2.20
7	SCCI	900	15	50	-	0.45	0.1	1.0	1.0	1.0	0.5	2.0	2.20
8	SCCI	900	30	50	-	0.45	0.1	1.0	1.0	1.0	0.5	2.0	2.20
9	RCCI	1000	30	50	12.8	0.45	0.1	1.0	1.0	1.0	0.8	1.2	1.25
10	SCCI	1000	30	50	-	0.45	0.1	1.0	1.0	1.0	0.8	1.2	1.25

3 Results and Discussions

Figure 4 shows the temporal evolutions of mean pressure, $\overline{p}$, and mean HRR, $\overline{q}$, during the first- and second-stage ignition of 0-D and 2-D DNS cases at three different T_0. Several points are noted from the figure. First, compared to SCCI, the overall combustion of RCCI are more advanced in time regardless of T_0 as such τ_{ig} of RCCI is much shorter than those of SCCI. Generally, mixtures of high reactivity with very short τ_{ig}^0 auto-ignite first, and then successfully develop intro deflagrations which subsequently advance the overall combustion and distribute the mean HRR over time, thereby reducing the peak $\overline{q}$.

Second, the effects of PRF and/or ϕ stratification on reducing the peak $\overline{q}$ are nearly eliminated when T_0 lies in the high temperature regime. It is because the difference in ignition delays caused by variations in PRF and/or ϕ is significantly reduced as shown in Fig. 3. As a result, the overall combustion is more likely to occur by spontaneous auto-ignition as readily observed in Fig. 5 (Cases 9–10).

Third, T_0 in the NTC regime has positive effects on enhancing the overall combustion of both RCCI/SCCI. However, the ignition characteristics of RCCI are affected more by the NTC regime than SCCI. The overall combustion of RCCI occurs much earlier and its combustion duration and the peak $\overline{q}$ are wider and smaller, respectively compared to the corresponding SCCI cases. The prolonged combustion durations are attributed to deflagrations with low-speed developed in RCCI than in SCCI. As shown in Fig. 5 (Cases 1–2, 5 and 8), 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 SCCI. For both RCCI/SCC, with T_0 in the NTC regime, PRF and/or equivalence ratio stratifications play a first-order effect on adjusting τ_{ig}. As readily seen in Fig. 4e, τ_{ig} is slightly changed with increasing T' from 0-30 K (Cases 3-5 and 6-7).

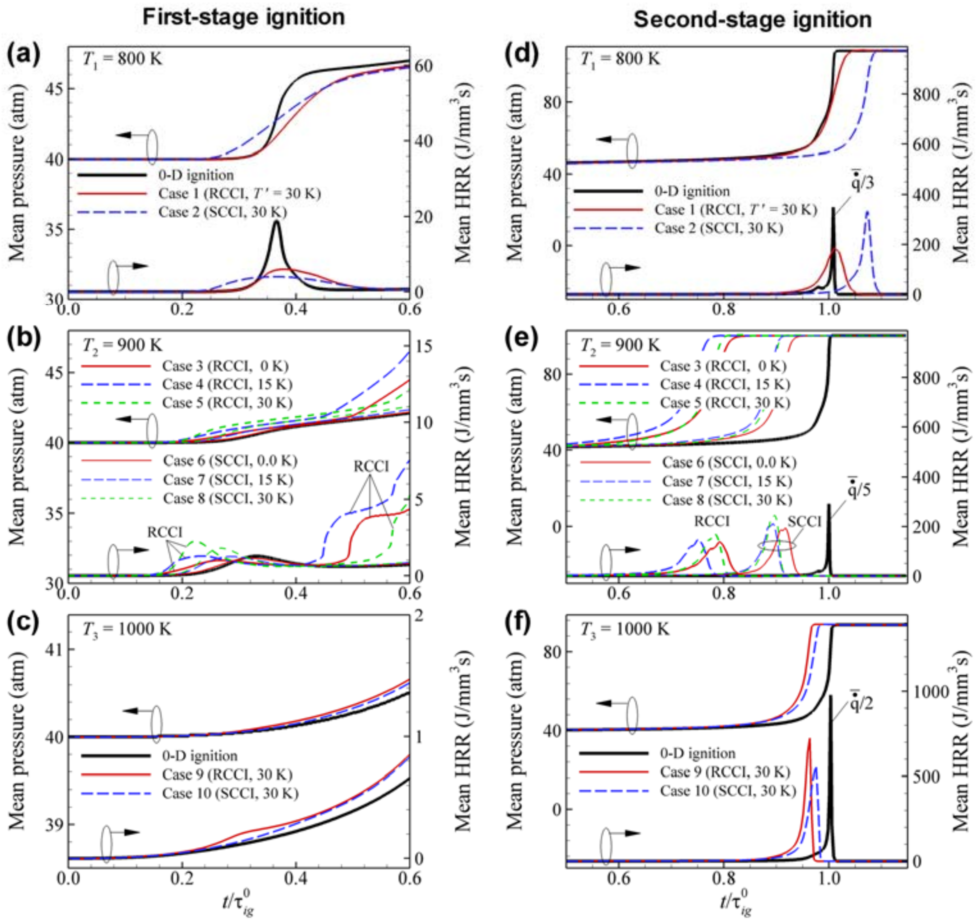

Figure 4. Temporal evolutions of the mean pressure and mean HRR for the cases with T_0 = 800 K (a & d), T_0 = 900 K (b & e), and T_0 = 1000 K (c & f) during the first- (left) and second-stage (right) ignition.

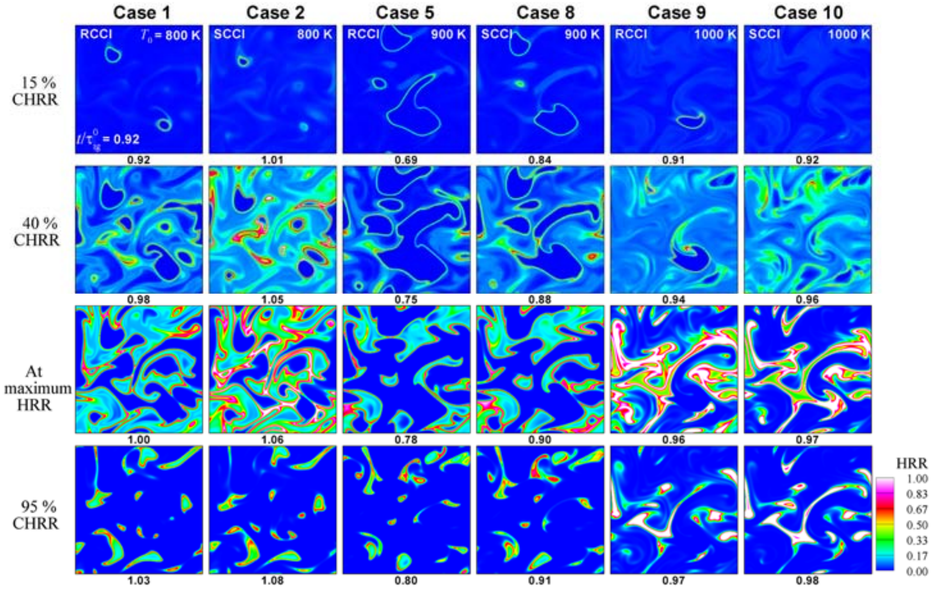

Figure 5. Isocontours of normalized HRR for the cases with T_0 = 800 K (Case 1–2), T_0 = 900 K (Case 5 & 8), and T_0 = 1000 K (Case 9–10) (from left to right) at times of 15% (first row), 40% (second row), and 95% (last row) cumulative mean HRR and at the maximum HRR (third row).

4 Conclusions

A comparative DNS study of RCCI and SCCI combustion with T_0 within and outside the NTC regime was conducted using a 116-species reduced PRF mechanism. The RCCI concept uses two different reactivity fuels (*iso*-octane is less reactive and *n*-heptane is highly reactive); while the SCCI concept uses a single fuel with a two-stage ignition fuel, PRF50. It is found that (1) compared to SCCI, the overall combustion of RCCI are more advanced in time regardless of T_0, (2) the effects of PRF and/or ϕ stratification on reducing the peak $\bar{q}$are nearly eliminated when T_0 lies in the high temperature regime, (3) T_0 in the NTC regime has positive effects on enhancing the overall combustion of both RCCI/SCCI. These results suggest the RCCI concept is better than SCCI in manipulating the overall combustion: more flexible in adjusting ignition timing, controlling the rate of heat release, and promisingly extending to a higher load.

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