DNSs of the Ignition of a Lean *n*-Heptane/Air Mixture under SCCI Conditions: A Parametric Study

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1 Introduction

Homogeneous-charge compression ignition (HCCI) engines have emerged as one of the most probable alternatives to conventional gasoline and diesel engines, providing high diesel-like thermal efficiency and avoiding excessive NOx and particulate emissions. However, the development of real HCCI engines encounters two remaining issues: excessive pressure-rise rate (PRR) and ignition-timing control [1-8].

One of the most effective methods to overcome these issues is thermal stratification of the in-cylinder fuel/air mixture, which can provide a smooth combustion process under high-load conditions by changing the combustion mode from spontaneous auto-ignition into a mixed combustion mode of spontaneous auto-ignition and deflagration. In a 2-D DNS study of the ignition of a thermally stratified *n*-heptane/air mixture under HCCI conditions, it was found that the temporal evolution of ignition of the mixture exhibits different behavior at different mean temperatures, T_0; and the overall combustion shows a non-monotonic behavior with increasing T' when T_0 lies within the NTC regime [2].

Another promising remedy is stratified-charge compression ignition (SCCI) combustion, which introduces a certain degree of fuel inhomogeneities. In practice, fuel-stratified mixture can be achieved by multiple high-pressure injectors with precisely-controlled injection timing. In two-stage injection, for instance, the main portion of fuel is first supplied during the intake stroke using a port fuel injector to generate relatively-homogeneous fuel/air mixture and additional fuel is then directly injected during the late compression stroke or near the TDC to introduce a certain degree of fuel stratification [4].

Due to the evaporation cooling effect of directly-injected fuel, thermal inhomogeneities can coexist with fuel stratification in SCCI combustion. Under such conditions, however, it is still questionable whether locally-richer mixtures with lower temperature or locally-leaner mixtures with higher temperature auto-ignite first. Several experimental studies reported that for partial fuel stratification, locally-richer mixtures are more likely to ignite first and then, combustion wave propagates towards adjacent leaner mixtures, thereby leading to a sequential ignition process. Wolk et al. found from their simulations [7] that the ignition of the stratified charge proceeds from relatively-leaner mixtures with high temperature to relatively-richer mixtures with low temperature at an intake pressure of 1 bar; however, the order of sequential auto-ignition events is reversed at an intake pressure of 2 bar. This non-monotonic ignition behavior is believed to be relevant to the low- and intermediate-temperature chemistry as the non-monotonic ignition delays observed in [2] with different mean temperatures in/near the NTC regime.

The objective of the present study is, therefore, to provide a better understanding of the effects of different T_0 within/near and outside the NTC regime together with both TP and ϕ' on the ignition characteristics of practical hydrocarbon fuel/air mixture under relatively-high pressure. 2-D DNSs are performed by varying four different key parameters: (1) mean temperature, (2) temperature fluctuation, (3) equivalence ratio fluctuation, and (4) spatial correlation between T and ϕ fields. In this study, *n*-heptane is adopted as a diesel-like fuel, which possesses a typically cool flame chemistry represented by the NTC regime under HCCI conditions. The details of the 58-species *n*-heptane/air reduced mechanism can be found in [2]

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. Twenty-three DNSs were carried out by varying three key parameters: (1) T_0 of 805, 933, and 1025 K, (2) T' of 15 and 60 K, and (3) ϕ' of 0.05 and 0.10. Among three initial mean temperatures, T_0 of 933 K lies in the middle of the NTC regime while T_0 of 805 and 1025 K lie slightly outside the NTC regime as shown in Fig. 1. Three T_0 have an identical 0-D ignition delay, τ_{ig}^0, of 1.5 ms. Therefore, the ignition characteristics of a *n*-heptane/air mixture can be investigated in three different regimes of the low-, intermediate-, and high-temperature chemistry.

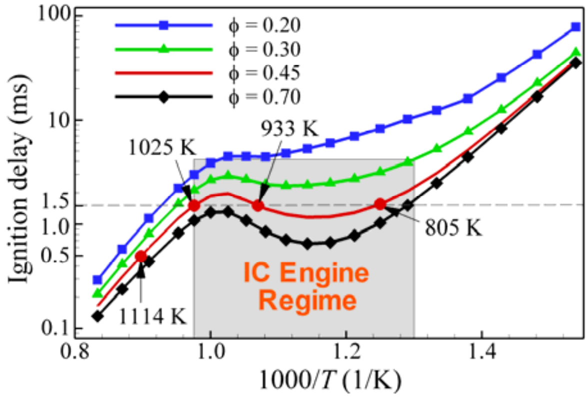

Figure 1. 0-D ignition delays of *n*-heptane/air mixtures as a function of initial temperature for different ϕ

At the TDC prior to the main auto-ignition event, different T–ϕ correlations may exist due to such factors as fuel delivery strategy, amount of EGR, intake charge heating, and wall heat loss. Here, two most-probable scenarios are examined: (1) uncorrelated T–ϕ fields resulting from the early direct injection in the one-stage injection in combination with EGR and turbulent mixing, and (2) negatively- correlated T–ϕ fields caused by the evaporative cooling of the second late-direct injection in the two-stage injection together with short mixing time. For completeness, cases with T' or ϕ' only are also elucidated and hence, three different initial T–ϕ correlations are considered in this study: (1) baseline cases with either T' or ϕ' only, (2) negatively-correlated T–ϕ distribution, and (3) uncorrelated T–ϕ distribution.

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 concentration stratifications, l_e, l_{Te}, and $l_{\phi e}$ are 1.25 mm for all the cases. The turbulence intensity, $u' = 0.83$ m/s, is selected such that the corresponding turbulence time scale, τ_t is comparable to τ_{ig}^0 ($\tau_t/\tau_{ig}^0 = 1.0$) and hence, most effective turbulent mixing of initial mixtures can be elucidated in the present DNS study. ϕ′

3 Results and Discussions

3.1 Effects of T′ or ff at different T₀: BL cases

Figure 2 shows the temporal evolutions of mean pressure, $\bar{p}$, and mean HRR, $\bar{q}$, of all BL cases. Note that cases with T_0 = 1025 K have no first-stage ignition due to their relatively-high T_0 as shown in Fig. 1. Several observations are noted from Fig. 2. First, $\bar{q}$ is more spread out over time and its peak is decreased with increasing T' or ϕ' for all cases regardless of T_0. As the degree of T' or ϕ' is increased, the deflagration mode of combustion rather than the spontaneous ignition mode prevails during the main combustion event and the mean HRR is significantly reduced due to the slow propagation speed of deflagrations compared to spontaneous ignition.

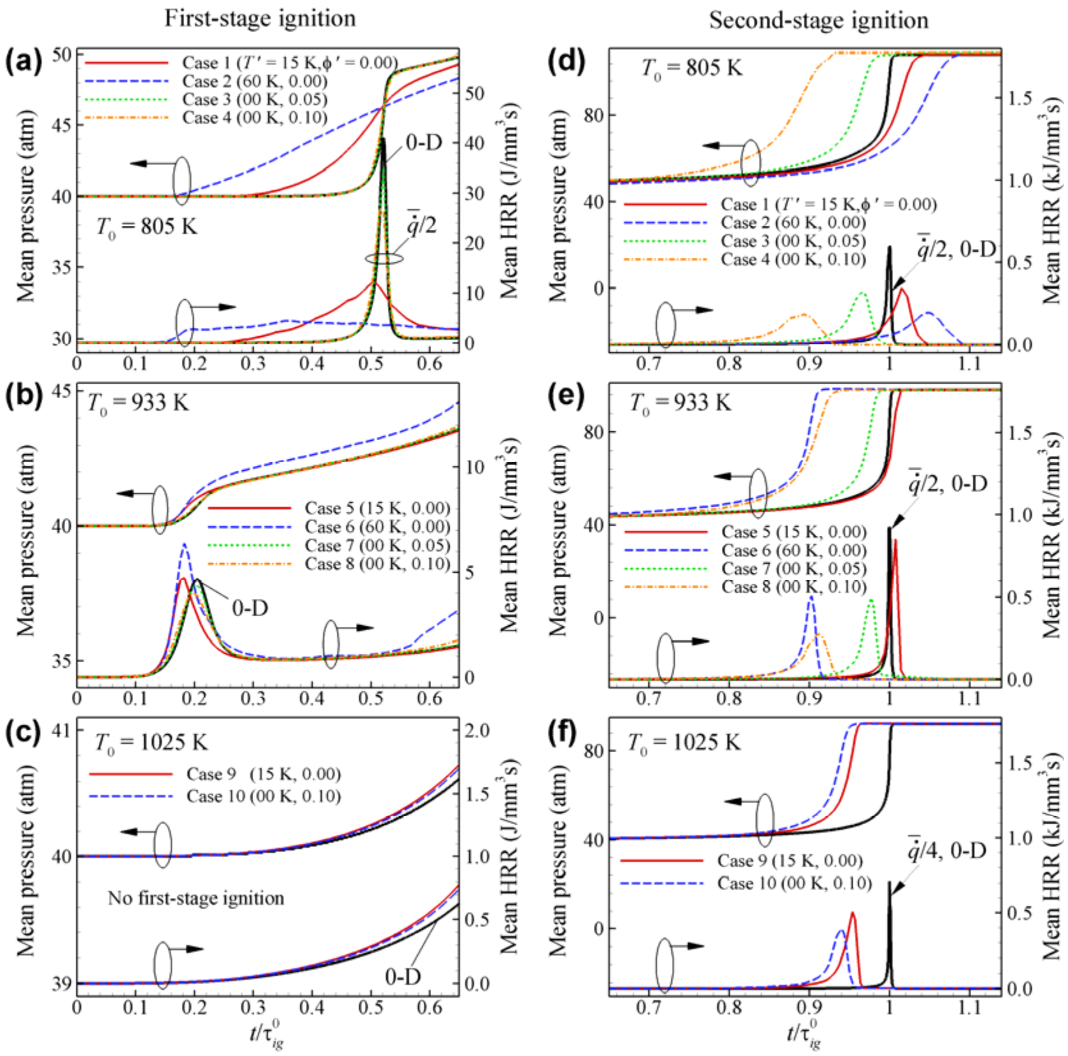

Figure 2. Temporal evolutions of the mean pressure and mean HRR for the BL cases (Cases 1−10).

Second, the ignition delay, τ_{ig}, behaves non-monotonically with T'(Cases 1, 2, 5, 6, and 9) at different T_0 but it is always decreased with increasing regardless of T_0 (Cases 3, 4, 7, 8, and 10). More specifically, as $T'$is increased, τ_{ig} is increased for low T_0 of 805 K; whereas, it is decreased for high T_0 of 1025 K. T_0 of 933 K, however, exhibits the combined effects of both low and high T_0 near the NTC regime: τ_{ig} is slightly increased with small T'while being decreased with large T'. Third, unlike the cases with T' only, the overall combustion of the baseline cases with ϕ' only (Cases 3, 4, 7, 8, and 10) is advanced in time and the duration of the main combustion is prolonged with increasing ϕ' regardless of T_0. It is also of interest to note that (1) when T_0 lies within the high temperature regime (Case 10), wherein the overall combustion is primarily governed by the high-temperature chemistry, fuel stratification becomes less effective in reducing the peak $\bar{q}$ and advancing τ_{ig}; (2) small T'induces quite similar result by large ϕ' in terms of the advancement of the overall combustion.

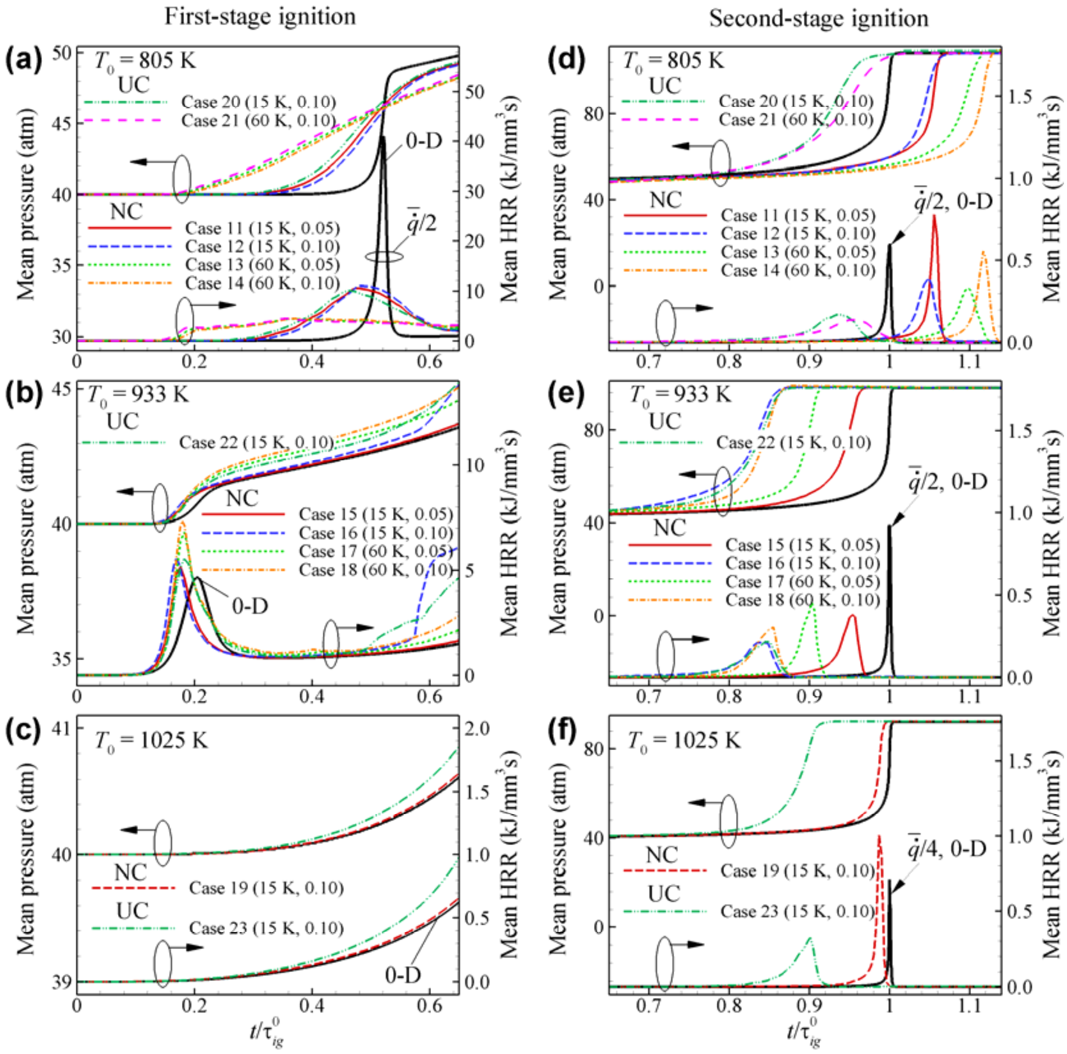

Figure 3. Temporal evolutions of the mean pressure and mean HRR for the NC and UC cases (Cases 11-23)

3.1 Effects of negatively-correlated T–ϕ fields: NC cases

Figure 3 shows the temporal evolutions of mean pressure, $\bar{p}$, and mean HRR, $\bar{\dot{q}}$, of all NC and UC cases. Several points are also observed from Fig. 3. First, for the low and high mean temperature, the negative T–ϕ correlation has an adverse effect on the overall combustion in terms of HRR distribution; the peak $\bar{\dot{q}}$ is significantly increased compared to those of the BL cases with T' or ϕ' only, while the duration of the main combustion is reduced. In addition, the overall combustion is finished much later than that of the corresponding baseline case. For cases with T_0 = 805 K, the temporal advancement and distribution of the overall combustion caused by ϕ' only are almost eliminated and even further reduced by the NC T–ϕ fields. For cases with T_0 = 1025 K, however, the favorable effect of both T' or ϕ' only on the HRR distribution vanishes while the overall combustion is also finished later than that of the baseline cases.

Second, for cases with intermediate T_0 of 933 K, the NC T–ϕ fields has a positive effect on the overall combustion by spreading out $\bar{\dot{q}}$ over time and reducing the peak $\bar{\dot{q}}$. Specifically, for cases with the same T' of 15 K or 60 K (Cases 15-16 or Cases 17-18), the overall combustion is more advanced in time and $\bar{\dot{q}}$ is more distributed over time with increasing ϕ', thereby reducing the peak $\bar{\dot{q}}$. To further elucidate the ignition characteristics of the NC cases at T_0 = 933 K, the instantaneous isocontours of HRR field are shown in Fig. 4. For Case 16, deflagration waves emanate from nascent ignition kernels much earlier than those for the other cases because the shortest τ_{ig}^{0} in Case 16 is smaller than those in other cases. For Cases 16 and 18, however, the temporal evolution of $\bar{\dot{q}}$ are not quite different. At time of 15% cumulative $\bar{\dot{q}}$, more corrugated deflagration waves are observed for Case 18 than 16, implying that Case 18 has more nascent ignition kernels which ultimately develop into deflagrations than Case 16.

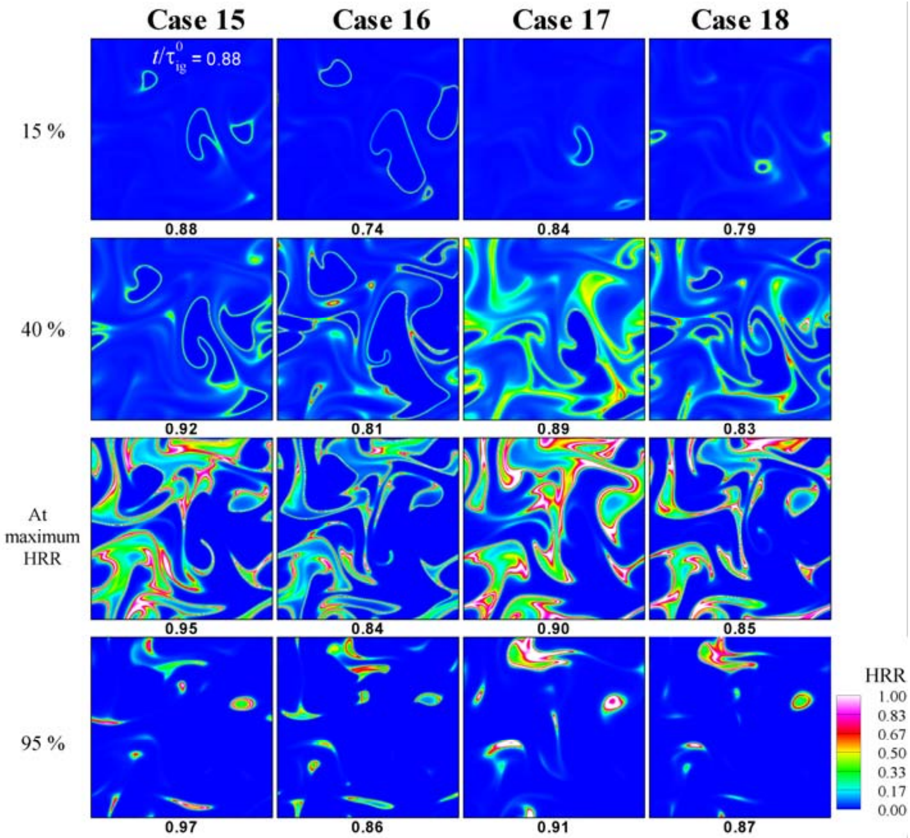

Figure 4. Isocontours of normalized HRR for Cases 15-18 (from left to right), at times of 15% (first row), 40% (second row), and 95% (last row) cumulative mean HRR and at the maximum HRR (third row).

For the cases with small ϕ' of 0.05 (Cases 15 and 17), however, large T' tends to advance the overall combustion and increase the peak $\bar{\dot{q}}$ slightly. In addition, for cases with the same ϕ', τ_{ig} for the NC cases are shorter than those of the corresponding BL cases with ϕ' only (Cases 8 and 9). These results imply that the NC $T\!-\!\phi$ fields at intermediate T_0 within the NTC regime have a synergistic effect on advancing the overall combustion and smoothing out the PRR and HRR under high-load HCCI combustion.

3.3 Effects of uncorrelated $T\!-\!\phi$ fields: UC cases

Several observations for UC cases can also be made from Figs. 3. First, unlike the NC cases, the overall combustion of all UC cases is more advanced in time and the duration of significant heat release is further increased regardless of T_0 compared to their corresponding τ_{ig}^{0}. Second, for cases with T_0 = 805 K (Cases 20 and 21), the temporal distribution of the mean HRR by uncorrelated $T\!-\!\phi$ field becomes more significant than the corresponding BL cases with ϕ' only (Cases 3 and 4), which is primarily attributed to the wider range of ignition delay of the UC cases. In the same context, uncorrelated large T' or ϕ' in Case 21 tend to retard the overall combustion compared to Case 4 with ϕ' only. The occurrence of ignition kernels and their development into deflagrations happens at the same time due to their similar fastest ignition delay. However, it takes more time to consume the whole fuel/air mixture of Case 21 with wide range of ignition delay than does Case 4 with relatively narrow range of ignition delay. Third, for cases with T_0 = 933 K (Case 22) and 1025 K (Case 23), the uncorrelated $T-\phi$ fields advance the overall combustion and spread out the mean HRR compared to the BL cases with T' or ϕ' only, which is also attributed to the shorter fastest ignition delays and wide range of ignition delay in the initial fuel/air mixture. In either way, the uncorrelated $T-\phi$ distribution has a synergetic effect in preventing excessive PRR by temporally distributing $\bar{\dot{q}}$ compared to the BL cases with T' or ϕ' only.

In summary, three key points relevant to HCCI combustion in the high temperature regime can be deduced: (1) the overall HCCI combustion is more sensitive to T' than ϕ', (2) uncorrelated $T-\phi$ fields inherently existing in an HCCI engine cylinder can advance the overall combustion in time by the synergetic effect of T' or ϕ' correlation, and (3) the effect of NC $T-\phi$ fields on the overall HCCI combustion is limited and not that significant compared to that in the NTC regime.

4 Conclusions

The ignition characteristics of thermally- and/or compositionally-stratified lean *n*-heptane/air mixture under HCCI conditions were investigated by performing 2-D DNSs with a 58-species reduced mechanism. It was found that (1) for the BL cases with ϕ' only, the overall combustion occurs more quickly and the mean HRR increases more slowly with increasing ϕ' regardless of T_0, however, for the BL cases with T' only, the overall combustion is retarded/advanced in time with increasing T' for low/high T_0 relative to the NTC regime, while shows the combined effects of both low and high T_0 for intermediate T_0 within the NTC regime; (2) for the NC cases, the negative $T-\phi$ correlation has an adverse effect on the overall combustion at low and high T_0, while for intermediate T_0 within the NTC regime, the NC $T-\phi$ fields has a synergistic effect on the overall combustion by spreading out $\bar{\dot{q}}$ over time and reducing the peak q; (3) for the UC cases, the mean HRR is more distributed over time and the overall combustion is more advanced in time.

These results suggest that an appropriate combination of T' and ϕ' together with a well-prepared $T-\phi$ distribution can provide a smooth ignition process and control ignition-timing in homogeneous charge compression-ignition (HCCI) combustion.

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