불균일한 온도 및 화학구성을 지닌 정상헵탄/공기 혼합물의 점화에 미치는 NTC영역의 효과

Minh Bau Luong* · 유광현* · 유춘상*†

Effects of the NTC Regime on the Ignition of a Lean *n*-Heptane/Air Mixture with Temperature and Composition Inhomogeneities

Minh Bau Luong*, Kwang Hyeon Yu*, Chun Sang Yoo*†

ABSTRACT

The effect of the negative temperature coefficient (NTC) on the ignition of a stratified lean *n*-heptane/air mixture of temperature and equivalence ratio was investigated using 2-D direct numerical simulations (DNSs) with a 58-species reduced mechanism. It was found that for T_0 in the NTC regime, fuel stratification is more effective than thermal stratification in controlling the ignition delay and mitigating the heat release rate (HRR). One of the key finding in this study is that for the intermediate T_0, the overall combustion becomes more advanced and mean heat release rate (HRR) is temporally more distributed with increasing ϕ' regardless of the negatively-correlated $T-\phi$ relations. It is primarily because the deflagrative mode prevails at the reaction fronts for large ϕ' and hence the combustion occurs subsequently, rendering mean HRR more distributed over time.

Key Words: DNS, HCCI, SCCI, *n*-heptane mechanism, composition inhomogeneities

Stratified-charge compression ignition (SCCI) combustion, one of variants of HCCI combustion, has been recently subject to being investigated by the engine community and shows promising potential in controlling precisely the combustion timing and preventing a rapid pressure rise rate (PRR), thereby offering to extend to higher load of HCCI combustion [1-2]. It was found that thermal stratification (TS) of in-cylinder fuel/air mixtures can offer a smooth combustion under high-load conditions by changing the combustion mode from spontaneous auto-ignition into a mixed mode of spontaneous and deflagrative combustion [3-7].

The effect of the NTC regime on the ignition of a lean *n*-heptane/air mixture with different means and variances of temperature was elucidated by Yoo et al using 2-D DNSs [3]. It revealed that ignition characteristics of two-stage ignition fuels can be significantly changed with different mean temperatures in the NTC region.

Recently, by using 2-D DNSs, Luong et al [4] has elucidated the combustion characteristics of a biodiesel/air mixture with both temperature and composition stratifications. However, the biodiesel/air mixture exhibits a relatively-weak NTC behavior and just one initial mean temperature, T_0, was investigated. Hence a comprehensive understanding of effects of different T_0 within the NTC regime on the ignition characteristics of large hydrocarbon/air mixtures exhibiting two-stage ignition under SCCI conditions is still elusive.

The scope of the present study, therefore, is to provide an better understanding of the influence of the NTC regime on the ignition characteristics of a practical hydrocarbon fuel/air mixture with $T-\phi$ stratifications at distinctive T_0 under elevated pressure. The 2-D DNSs are performed by varying three key parameters: (1) different T_0 (2) temperature RMSs, and (3) equivalence ratio RMSs. In this

* 유니스트 기계 및 원자력공학부
† 연락저자, csyoo@unist.ac.kr
TEL : (052)217-2322 FAX : (052)217-2308

study, n-heptane is adopted as a diesel-like fuel, which possesses a strong cool flame chemistry under HCCI conditions. More details of n-heptane/air reduced mechanism can be found in [3].

The Sandia DNS code, S3D, was used with a 58-species reduced n-heptane mechanism for HCCI simulations. For all DNSs, mean equivalence ratio, ϕ_0 and the initial uniform pressure, p_0, are 0.45 and 40 atm, respectively. Twenty three cases are performed by varying three key parameters: (1) T_0 of 805 K, 933 K, and 1025 K; (2) T' of 15 K and 60 K; and (3) ϕ' of 0.05 and 0.10. Note that these T_0 have the identical 0-D ignition delay, τ_{ig}^0 = 1.5 ms, where T_0= 805 K and 933 K lie within, while T_0 = 1025 K lies slightly outside the NTC regime. The turbulence intensity, u'= 0.83 m/s, length scale, l_e= 1.25 mm, the turbulence time scale, τ_t= 1.5 m/s, and the most energetic length scale of the temperature fluctuation, l_{Te}= 1.25 mm are specified for all cases. Three distinctions of $T-\phi$ correlations are considered: (1) baseline cases (BLs) with the variance of either T or ϕ, (2) negatively-correlated (NC) $T-\phi$, and (3) uncorrelated (UC) $T-\phi$ distributions. The computational domain is a 2-D square box with each size, L, of 3.2 mm, discretized with grid size of 2.5 μm.

Figure 1 shows the temporal evolutions of the mean pressure, $\bar{p}$, mean HRR, $\bar{\dot{q}}$. and the corresponding 0-D homogeneous ignitions of three mean temperatures. In the fist parametric study, to isolate the thermal from fuel effect, BLs with either T'(Cases 1-5) or ϕ' alone (Cases 6-10) are separately examined as shown in Fig. 1a-c. Several observations can be noted from Fig. 1a-c. First, for BLs with T'only, as T' is increased, τ_{ig} retards for the low T_0 of 805 K; while advances for the high T_0 of 1025 K. For the intermediate T_0 of 933 K, however, τ_{ig} slightly increases with small T', while decreases with large T'. It is because Cases 3-4 (T_0 = 933 K) exhibit the combined effects of both low and high T_0 near the NTC regime. Second, unlike the cases with T'only, the overall combustion of Cases 6-10 with ϕ' alone occurs quickly and the combustion duration prolongs with increasing ϕ' regardless of the difference in the initial T_0. As a result, $\bar{p}$ increases slowly and $\bar{\dot{q}}$ is temporarily spread out more as ϕ' is increased. However, it seems that when the initial T_0 is increased from (805 K → 933 K→ 1025 K), fuel stratification becomes less effective in reducing the peak $\bar{\dot{q}}$ and τ_{ig} even with high ϕ' = 0.10. Generally, for a mixture with large T' and/or ϕ', the onset of combustion is initiated by the auto-ignition of locally-hotter and/or locally-richer mixture, thereby nascent ignition kernels are developed and then become flame-like fronts, which propagate and consume most of the unburnt-air/gas mixtures as deflagration waves; subsequently, the end-gas mixture is auto-ignited at the end of combustion due to compression heating effects. Hence, the deflagration becomes the predominant combustion mode with increasing $T'$and/or ϕ'. These results are qualitatively similar to those of previous studies that [3-4].

In the second parametric study, the competitive effect of $T'$and ϕ'on the overall n-heptane/air mixture under HCCI conditions is investigated as shown in Fig. 1d-f with different NC $T-\phi$ fields, which captures one of the most probable $T-\phi$ correlations that can be achieved by a late-direct injection. Basing on T_0, two key points are noted from the figure. First, for the low or high T_0 of 805 K or 1025 K, the negative $T-\phi$ correlations have an adverse effect on the overall combustion, that is, the peak $\bar{\dot{q}}$ is increased more and the combustion is retarded further relative to the corresponding BLs with T' only. Second, for the intermediate T_0 of 933 K, NCs of $T-\phi$ fields offer a positive influence in advancing τ_{ig} and reducing the peak PRR and HRR. This ignition characteristic is one of key findings in the present study. Another observation is that with the same ϕ', τ_{ig} of NCs are shorter than those of the corresponding Bls with ϕ'only (Cases 8-9), implying that NCs of $T-\phi$ distributions combined with the intermediate T_0 have a synergistic influence on decreasing τ_{ig} and temporally speading out the PRR and

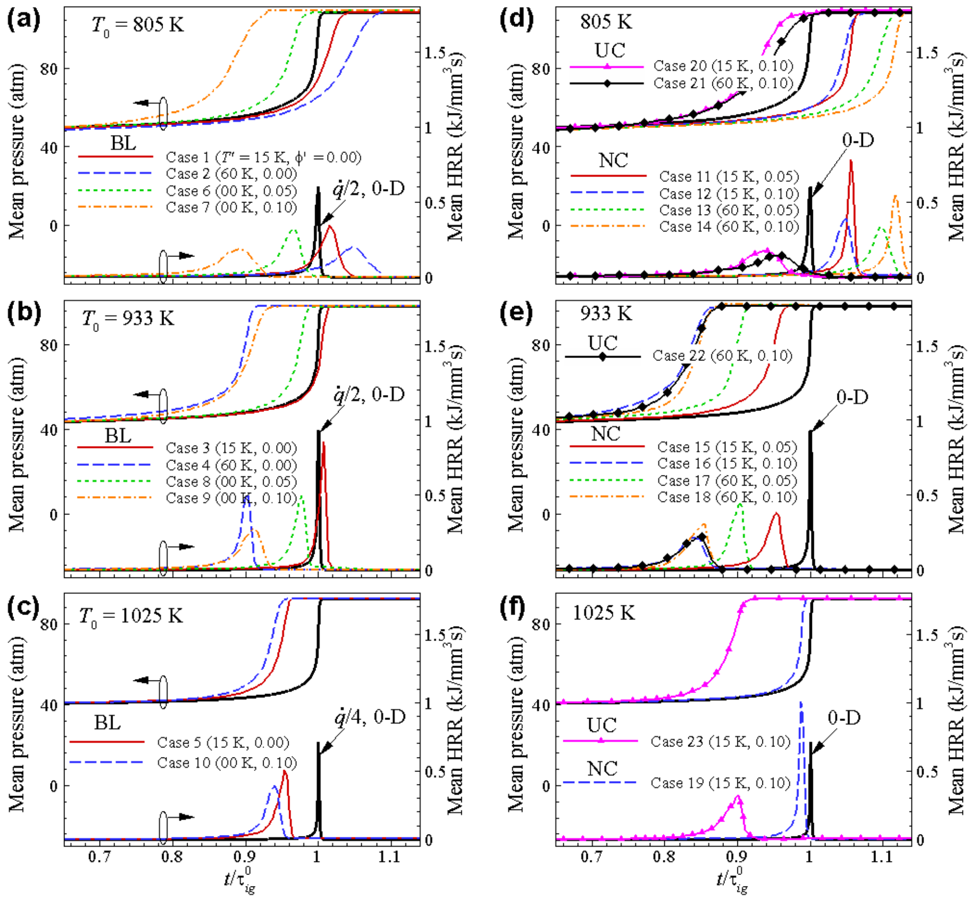

Fig. 1 Temporal evolution of mean pressure and HRR for Case1-23. Thick black lines represent the corresponding 0-D homogeneous ignition of three different T_0 of 805 K, 933 k, and 1025 K.

HRR under the high-load HCCI combustion.

In the third parametric study, another high probability of the $T-\phi$relations near the TDC is randomly-distributed $T-\phi$ fields caused by port fuel injection or early-direct injection together with heat-transfer management. From the previous study [4] it was found that for the intermediate T_0 of a biodiesel/air mixture with UC $T-\phi$ fields under HCCI combustion, as ϕ' is increased, the overall combustion occurs rapidly and the combustion duration is elongated by a sequential ignition event thereby reducing the peak HRR. Therefor, a few additional cases of UC $T-\phi$ distributions (Cases 20-23) are examined as shown in Fig. 1d-f to provide a more in-depth understanding of the combined effect of the NTC regime and uncorrelated stratification in T and ϕ on the overall HCCI combustion. Two main points can be made from Fig. 1d-f. First, large ϕ' causes an advancement in τ_{ig} regardless of three different T_0 or the effect of the NTC regime. Second, the combination of $T-\phi$ stratification induces a synergistic effect on the overall combustion by distributing more $\bar{p}$ and $\dot{\bar{q}}$ in time. As readily seen in Fig. 1d-f, interestingly, ϕ' exhibits a first-order effect over T' in adjusting τ_{ig}. Moreover, as T_0 is increased, the synergistic effect of thermal and fuel stratification becomes more sensitive in adjusting combustion timing (see Cases 22-23 in Fig. 1e-f).

To provide a qualitative assessment discerning different combustion modes, the isocontours of the HRR field, $\dot{q}$, of distinctive cases (BL, NC, and UC cases) with identical T' = 60 K and/or ϕ' = 0.10 at maximum HRR

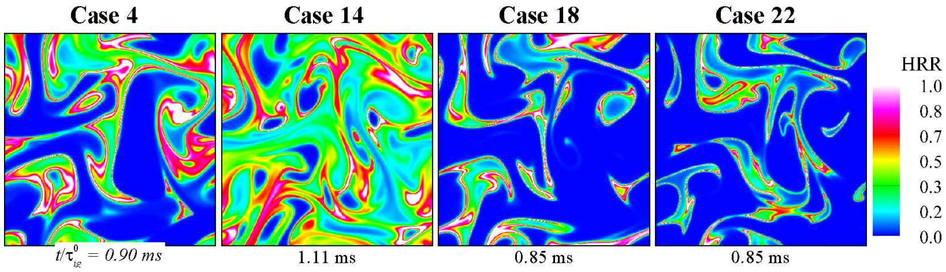

Fig. 2 Isocontours of normalized HRR at t of maximum heat release for Cases 4, 14, 18, and 22.

are chosen as shown in Fig. 2. Note that for the cases with different T_0, the HRR fields are normalized by its corresponding maximum HRR $\dot{q}_m^0$ of the 0-D homogeneous ignition. For Cases 4 (T' = 60 K), although thin reaction sheets are developed as deflagration at early occurrence of combustion, they propagate outwards quickly to burn out the remaining charge as a mixde mode of spotaneous ignition and deflagrative waves with high $\dot{q}$ zones (white and red colors) prevailing in relative-broad areas as spontaneous ignition. However, thanks to the synergistic effect of high T' with ϕ' for Case 18 and 22 (with NC and UC $T-\phi$ correlations, respectively), low $\dot{q}$ (green color) occurs in much broader areas along with moderate $\dot{q}$ (white and red color) in thin sheets propagating subsequentially as deflagrative combustion. Consequently, the overall combustion is enhanced significantly by prolonging combustion duration with a sequential ignition event, effectively reducing the peak HRR and smoothing out the PRR. On the contrary, for Cases 14 with the NC $T-\phi$ correlation), HRR occurs volumetrically as spontaneous auto-ignition nearly in the absence of flame front-like propagation. As such the overall combustion is retarded by turbulent mixing and occurs simultaneously by spontaneous auto-ignition.

2-D DNSs of a lean n-heptane/air mixture at high pressure were performed using a 58-species reduced mechanism to investigate the effects of the NTC regime and $T-\phi$ stratifications on the ignition characteristics of n-heptane HCCI combustion. It is found that (1) for T_0 in the NTC regime, fuel stratification plays an predominant role in adjusting the ignition timing and alleviating the heat release rate (HRR); (2) the overall combustion of the intermediate T_0 with the NC $T-\phi$ distributions becomes advanced and hence $\bar{\dot{q}}$ is spread out considerably with increasing ϕ'.

These results suggest that a harmonious combination between T_0 and stratification of temperature and composition under a well-designed $T-\phi$ field can prevent an excessive combustion rate under the high-load and regulate effectively the timing of combustion in HCCI engines.

Acknowledgements

This study was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. 2011-0008201). MBL was also supported by BK21Plus funded by the Ministry of Education.

References

[1] J. Dec, *Proc. Combust. Inst.*, 32 (2009) 2727-2742.
[2] M. Yao, Z. Zheng, and H. Liu, Prog. Energy Combust. Sci, 35 (2009) 398 - 437
[3] C .S. Yoo, T. Lu, J. H. Chen, and C. K. Law, *Combust. Flame*, 158 (2011) 1727-1741.
[4] M. B. Luong and C. S. Yoo, 한국연소학회 제47회 추계학술대회. 부산, 2013.
[5] C. S. Yoo, Z. Luo, T. Lu, H. Kim, and J. H. Chen, *Proc. Combust. Inst.*, 34 (2013) 2985
[6] M. B. Luong, Z. Luo, T. Lu, S. H. Chung, C. S. Yoo, Combust. Flame 160 (10) (2013) 2038-2047
[7] G. Bansal and H.G. Im, *Combust. Flame* 158 (2011) 2105-2112.