A DNS study of the ignition of lean PRF/air mixtures with temperature inhomogeneities under high pressure and intermediate temperature

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Abstract

Two-dimensional direct numerical simulations (DNSs) of ignition of lean primary reference fuel (PRF)/air mixtures at high pressure and intermediate temperature near the negative temperature coefficient (NTC) regime were performed with a 116 species-reduced mechanism to elucidate the effects of fuel composition, thermal stratification, and turbulence on PRF homogeneous charge compression-ignition (HCCI) combustion. In the DNSs, temperature and velocity fluctuations are superimposed on the initial scalar fields with different PRF compositions. In general, it was found that the mean heat release rate increases slowly and the overall combustion occurs rapidly with increasing thermal stratification regardless of the fuel composition. In addition, the effect of the fuel composition on the ignition characteristics of PRF/air mixtures was found to be significantly reduced with increasing thermal stratification. Chemical explosive mode (CEM) and displacement speed analyses verified that nascent ignition kernels induced by hot spots due to a high degree of thermal stratification usually develop into deflagrations rather than spontaneous auto-ignition at reaction fronts and as such, the mean heat release rate becomes more distributed over time. These analyses also revealed that the fuel composition effect vanishes as the degree of thermal stratification is increased because the deflagration mode of combustion, of which propagation characteristics are nearly identical for different PRF/air mixtures, becomes more prevailing with increasing degree of thermal stratification. Ignition Damköhler number was proposed to quantify the successful development of deflagrations from nascent ignition kernels; for cases with large ignition Damköhler number, turbulence with high intensity and short timescale can advance the overall combustion by increasing the overall turbulent flame area instead of homogenizing initial mixture inhomogeneities.

Keywords: Homogeneous charge compression ignition (HCCI), Direct numerical simulation (DNS), Primary reference fuel (PRF), Negative temperature coefficient (NTC) regime, Ignition

24 **1. Introduction**

25 The fundamental ignition characteristics of various fuel/air mixtures under lean, dilute, elevated
26 pressure, and relatively low temperature have been widely investigated due to their practical rel-
27 evance to homogeneous charge compression-ignition (HCCI) engine combustion [1–14]. An HCCI
28 engine and its many variants have been considered as one of the most probable alternatives to the
29 conventional internal combustion engines due to its potential to provide high diesel-like efficiency
30 with very low pollutant emissions [1–14]. However, the development of prototype HCCI engines
31 remains challenging because of their significant drawbacks in preventing an excessive pressure rise
32 rate (PRR) under high-load conditions and controlling precise ignition timing of HCCI combustion.
33 In general, the excessive PRR occurs due to volumetric auto-ignition throughout an HCCI engine
34 cylinder. Moreover, HCCI engines have no explicit ignition method such that ignition timing in
35 HCCI combustion is primarily governed by the chemical kinetics of fuel/air mixture, which depend
36 highly on overall mixture composition, temperature, and pressure. Therefore, there have been
37 many attempts to control the ignition timing and to alleviate the excessive PRR in HCCI com-
38 bustion by applying different fuel injection strategies, fuel preparation, and thermal management
39 including exhaust gas recirculation (EGR) [1–14].

40 Several computational studies of HCCI combustion using multi-dimensional direct numerical
41 simulations (DNSs) have been conducted to elucidate the fundamental combustion characteristics
42 of various fuel/air mixtures under HCCI conditions including hydrogen [15–19], dimethyl ether
43 (DME) [20, 21], *n*-heptane [22], *iso*-octane [23], primary reference fuel (PRF) [24], ethanol [25],
44 and biodiesel [26]. From these studies, the general characteristics of HCCI combustion have been
45 elucidated; thermal stratification in an HCCI engine cylinder can spread out the PRR under
46 high-load conditions by changing a combustion mode of spontaneous auto-ignition into a mixed
47 combustion mode of spontaneous auto-ignition and deflagration [15–18, 22, 23]. In the presence
48 of large temperature fluctuations, auto-ignition of hotter mixtures first occurs and evolves into
49 deflagration waves, which spread to the unburnt mixtures sequentially until the remaining charge

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50 auto-ignites simultaneously. In general, the speed of the deflagration waves is much less than that
51 of the spontaneous auto-ignition fronts and hence, the overall combustion is temporally spread out,
52 resulting in a reduction of peak PRR.

53 In many previous DNS studies [15–19], the ignition characteristics of hydrogen/air mixtures ex-
54 hibiting only one-stage ignition were investigated and as such, the effect of the negative-temperature
55 coefficient (NTC) regime on HCCI combustion was not appreciated. The NTC regime usually ap-
56 pears as a result of the low-temperature oxidation of large hydrocarbon fuels exhibiting two-stage
57 ignition. The effect of the NTC regime on HCCI combustion was first investigated by Yoo et al.
58 [22] using 2-D DNSs of the ignition of a lean *n*-heptane/air mixture with different means and root-
59 mean-squares (RMSs) of temperature. Recently, El-Asrag and Ju [20, 21] investigated the effects
60 of EGR and temperature/mixture stratification on the ignition of synthetic DME by adding H_2O_2
61 and NO to the initial mixtures. Bansal and Im [18], and Bhagatwala et al. [25] also investigated
62 the effect of the equivalence ratio fluctuations on HCCI combustion and found that the equivalence
63 ratio fluctuations enhance HCCI combustion together with temperature fluctuations when they are
64 uncorrelated and retard it when negatively correlated.

65 It is of interest to note that in a previous DNS study of the ignition of PRF/air mixtures at
66 elevated pressure and high temperature [24], it was found that the effect of different fuel composition
67 on the overall combustion vanishes with increasing temperature inhomogeneities. This is primarily
68 attributed to the predominant deflagration mode of combustion at the reaction fronts and the
69 nearly-identical propagation characteristics of different PRF/air deflagrations. It was also found
70 that turbulence with large intensity and short timescale can effectively homogenize the initial
71 mixtures, rendering the overall combustion to occur by spontaneous auto-ignition.

72 However, the homogeneous ignition delays of different PRF/air mixtures under high pressure
73 and intermediate temperature conditions, which are more relevant to practical HCCI combustion,
74 show a big disparity among the mixtures (see Fig. 1) and hence, it may be expected that the
75 effect of fuel composition may not vanish even with large temperature fluctuations. Moreover,
76 the early phase of ignition of a fuel/air mixture with very large temperature fluctuation may not
77 be affected by turbulence [23]. In many previous studies [16, 17, 19, 22–24], it was found that
78 turbulence is likely to homogenize the initial mixtures in HCCI combustion and hence, retard its
79 overall combustion. On the contrary, it was also found [23, 25] that turbulence may enhance the

80 overall spark-assisted compression ignition (SACI) combustion. These DNS results imply that the
81 effect of turbulence on HCCI/SACI combustion may be inconclusive.

82 Therefore, the objective of the present study is to understand and compare the ignition char-
83 acteristics of different PRF/air mixtures at high pressure and intermediate temperature near the
84 NTC regime. For this purpose, we perform 2-D DNSs by varying three key parameters: 1) the
85 fuel composition, 2) the initial temperature fluctuation, and 3) the initial turbulence intensity.
86 Note that both of the initial temperature and composition fluctuations play an important role in
87 HCCI combustion [10, 26]; in general, the equivalence ratio fluctuations enhance HCCI combustion
88 together with temperature fluctuations when they are uncorrelated and retard it when negatively
89 correlated. In the present study, however, we focus only on the effects of temperature fluctua-
90 tions and turbulence rather than that of equivalence ratio fluctuations because large equivalence
91 ratio fluctuations may be equivalent to large temperature fluctuations if the initial temperature
92 of mixture is near or above the NTC regime. Note that PRF is a fuel mixture of pure *n*-heptane
93 and *iso*-octane; for instance, PRF80 is comprised of 80% *iso*-octane and 20% *n*-heptane by liquid
94 volume.

95 2. Numerical methods and initial conditions

96 For the present DNSs, the Sandia DNS code, S3D [27, 28], is used with a 116-species PRF/air
97 reduced chemistry [24]. S3D solves compressible Navier-Stokes, continuity, total energy, and species
98 continuity equations using a fourth-order, low storage, explicit Runge-Kutta method for time
99 integration [29] and an eighth-order central differencing scheme for spatial discretization [30] with
100 a tenth-order filter. CHEMKIN and TRANSPORT software libraries are linked with S3D to
101 calculate reaction rates and thermodynamic and mixture-averaged transport properties. Details of
102 the numerical algorithm and its implementation are provided in [27]. As in previous DNS studies
103 of HCCI combustion [22–24, 26], periodic boundary conditions are applied in all directions and as
104 such, ignition of PRF/air mixtures occurs at constant volume.

105 The skeletal and reduced mechanisms for PRF oxidation were developed for a previous DNS
106 study of ignition of PRF/air mixtures under HCCI condition [24] based on the detailed LLNL
107 mechanism [31, 32], using a strategy combining directed relation graph (DRG)-based methods,
108 isomer lumping, and timescale analysis [24, 33–36]. The skeletal and reduced mechanisms were

validated under various PRF composition, pressure, and temperature conditions. Readers are referred to [24] for details of the reduced mechanism.

For all DNSs, we adopted the initial uniform equivalence ratio, ϕ_0 , of 0.4, pressure, p_0 , of 40 atm, and mean temperature, T_0 , of 850 K, respectively. p_0 of 40 atm and T_0 of 850 K represent high pressure and intermediate temperature near the NTC regime to approximate the conditions in a hydrocarbon-fueled HCCI engine at the top dead center. Under the present initial conditions, the homogeneous ignition delays, τ_{ig}^0 , of PRF50 and PRF80 are found to be 2.5 and 6.3 ms, respectively. Henceforth, τ_{ig} represents the time at which the maximum mean heat release rate (HRR) occurs for all simulations. The superscript 0 denotes the 0-D simulation. A total of ten different DNSs were performed in two dimensions by changing the initial physical conditions: different fuel compositions; temperature fluctuation RMS, T' ; and turbulence velocity fluctuation, u' .

The initial turbulent flow field is prescribed by an isotropic kinetic energy spectrum function as in [15–17, 37–39]. The most energetic length scale of turbulence, l_e , is 1.25 mm. Note that the largest velocity fluctuations in real engines are about 5 m/s such that u' of 0.5 and 2.5 m/s adopted in the present study is quite comparable to that in real engines. Note also that the turbulence timescale in real HCCI engines is $\sim O(1 \text{ ms})$ such that the turbulence timescale in this study, defined as $\tau_t = l_e/u'$, is representative of HCCI combustion. Similar to the initial turbulence field, the initial temperature fluctuation is generated by a temperature spectrum function. For all cases, the most energetic length scale of the temperature fluctuation, l_{Te} , of 1.25 mm is selected such that identical l_e and l_{Te} can produce the most effective turbulent mixing as found in [23]. Table 1 shows the details of the physical and numerical parameters. Note that temperature and turbulence fields in the present study are uncorrelated as shown in Fig. 2.

From experiments of HCCI engine [40], it was found that T' is approximately 15 ~ 20 K without thermal management of initial mixture. Therefore, $T' = 60$ or 120 K considered in the present study is somewhat large compared to that in real engines. However, these large T' can be achieved through direct injection or delayed-fuel injection in HCCI combustion. Furthermore, the spark ignition in SACI combustion [23] and the injection of highly-reactive fuel into an engine cylinder in reactivity controlled compression ignition (RCCI) combustion [41] can significantly reduce the ignition timing as large T' in the present study, and hence, it is also important to understand the characteristics of HCCI combustion with large T' .

It is of interest to note that 2-D turbulence without vortex stretching and tilting is different from 3-D turbulence. However, it is nearly impossible to do a parametric 3-D DNS study due to its great computational expense and hence, it is still valuable to investigate HCCI combustion using 2-D turbulence with a wide range of spectrum of time- and length-scales by systematically varying important parameters such as temperature and equivalence ratio fluctuations. Moreover, it was found from previous studies [15–18, 22–24] that turbulent mixing plays a secondary role in HCCI combustion compared to temperature stratifications. In addition, it was found from [19, 25] that 3-D turbulence may retard/enhance the overall HCCI/SACI combustion slightly more than 2-D turbulence by homogenizing the initial mixtures/increasing turbulent flame area but its effect on overall HCCI/SACI combustion is not significant.

As in previous studies [22–24], a square box of $3.2 \times 3.2 \text{ mm}^2$ is chosen for the computational domain, which is discretized with 640 or 1280 grid points, N , for the cases in Table 1. In 2-D DNSs, the turbulent Reynolds numbers based on u' and the integral length scale for cases with $u' = 0.5$ and 2.5 m/s are 69 and 347, respectively. The corresponding Kolmogorov length scales, η_K , are approximately 17.5 and $5.3 \text{ }\mu\text{m}$, respectively. For all DNS cases, therefore, the Kolmogorov length scale is resolved with at least a grid point [42]. In addition, the thinnest reaction layers in 2-D DNSs are resolved with at least $12 \sim 18$ grid points and as such, turbulence and scalar fields are well resolved in the DNSs. All of the DNSs were performed either on the Cray XC30 at National Energy Research Scientific Computing Center or on the Cray XK7 at Oak Ridge National Laboratory.

3. Effect of fuel composition and T'

In the first parametric study, six different DNS cases (Cases 1–6) are simulated (see Table 1 for detailed parameters of the DNSs) to elucidate the combined effect of the initial fuel composition and temperature fluctuation on the ignition of lean PRF/air mixtures. Different degrees of temperature fluctuation for different PRF/air mixtures are chosen: i.e., $T' = 15, 60$, and 120 K .

3.1. Overall ignition characteristics

Figure 3 shows the temporal evolution of mean pressure, $\bar{p}$, mean HRR, $\bar{q}$, and mean PRR, $\bar{p}$, with different levels of temperature fluctuations for different PRFs (Cases 1–6), where “mean” represents the spatial average over the whole simulation domain. Note that the 0-D ignition delay

168 of the PRF50/air mixture ($\tau_{ig}^0 = 2.5$ ms) is chosen as the reference time; $\bar{q}$ for the cases with T'
 169 $= 15$ K and 0-D cases are divided by 5. Several ignition characteristics of the PRF/air mixtures
 170 are to be noted. First, $\bar{p}$ increases more slowly and $\bar{q}$ is more distributed over time with increasing
 171 T' for all fuel compositions, similar to the results in previous studies [15–17, 22–24]. Moreover,
 172 the shapes of the overall combustion for Cases 1 and 4 with small T' are nearly identical to the
 173 corresponding 0-D ignitions. This is because the PRF50/air and PRF80/air mixtures exhibit nearly
 174 constant ignition delays at intermediate temperatures around 850 K as shown in Fig. 1, implying
 175 that mixtures with small T' are not able to take any advantage of temperature fluctuations to
 176 advance the overall combustion [22, 24].

177 Second, overall combustion occurs rapidly and the peak $\bar{q}$ is reduced with increasing T' for the
 178 same PRF/air mixture, which results in prolonging the vigorous combustion phase. Similar results
 179 were also observed from the DNSs of hydrogen, *n*-heptane, *iso*-octane, and PRF HCCI combustion
 180 [16, 17, 22–24]. This is primarily attributed to the occurrence of deflagrations by the large degree
 181 of T' , leading to smoothing of $\bar{q}$ and fast occurrence of overall combustion. As discussed earlier,
 182 large T' generally induces a mixed mode of deflagration and spontaneous auto-ignition, while small
 183 T' leads to spontaneous auto-ignition throughout the entire domain.

184 Third, for cases with the same T' , the effect of fuel composition is significantly reduced with
 185 increasing T' . For cases with small T' (Cases 1 and 4), τ_{ig} increases significantly with increasing
 186 *iso*-octane volume percentage in the PRF as can be expected from their τ_{ig}^0 ; i.e., $\tau_{ig}^0 = 2.5$ and 6.3
 187 ms for PRF50 and 80, respectively. However, for cases with large T' (Cases 3 and 6), the difference
 188 between τ_{ig} of the PRF/air mixtures is significantly decreased; i.e., $\tau_{ig}/\tau_{ig}^0 = 0.6$ and 0.8 for PRF50
 189 and 80, respectively. This result implies that even at intermediate T_0 , the effect of different fuel
 190 compositions of PRFs on HCCI combustion may vanish with increasing T' , similar to the PRF
 191 HCCI combustion at high T_0 [24].

192 To further identify the overall combustion characteristics of the 2-D DNS cases, the temporal
 193 evolutions of the mean mass fractions of important species and the mean HRR are shown in Fig. 4
 194 for four representative cases (Cases 1, 3, 4, and 6) together with their corresponding 0-D ignitions.
 195 At the first stage ignition, reaction is initiated by the abstraction of H from a fuel molecule (RH)
 196 by O_2 ($RH + O_2 \rightarrow R + HO_2$), forming a cycle with $R + O_2 + M \rightleftharpoons RO_2 + M$ to produce
 197 H_2O and alkylperoxide, $O=ROOH$ [31, 32, 43, 44]. As such, HO_2 increases significantly while

198 *iso*-octane and *n*-heptane decreases rapidly during the first stage ignition of the 0-D ignitions as
 199 shown in Figs. 4a and d. This low-temperature reaction cycle comes to an end when temperature
 200 exceeds a certain value at which the competing reaction, $R + O_2 \rightarrow \text{olefin} + HO_2$, terminates the
 201 first stage ignition. Subsequent exothermic reactions start to generate olefin and H_2O_2 , increasing
 202 temperature slowly until the chain branching reaction, $H_2O_2 + M \rightarrow OH + OH + M$, becomes
 203 important [31, 32, 43, 44]. This reaction sequence proceeds rapidly until the increase of temperature
 204 becomes enough to initiate the high-temperature chain branching reactions, controlled by $H + O_2$
 205 $\rightarrow O + OH$. This overall description of the HCCI combustion can be readily found from the
 206 0-D ignitions (see Figs. 4a and d): H_2O_2 is first accumulated from the first stage ignition, and
 207 then vanishes with a rapid increase of OH during the second stage ignition, which indicates the
 208 importance of H_2O_2 in determining the second stage ignition delays.

209 It is also readily observed from Fig. 4 that the temporal evolutions of the important species
 210 in Cases 1 and 4 with small T' are nearly identical to those of the corresponding 0-D ignitions,
 211 which verifies the predominance of the spontaneous auto-ignition mode of combustion during the
 212 whole combustion. Unlike the cases with small T' , however, the overall combustion of Cases 3
 213 and 6 with large T' proceeds gradually without two-stage ignition characteristics; *iso*-octane and
 214 *n*-heptane are consumed more gradually; the production of CO and CO_2 are more distributed over
 215 time compared with those of the 0-D ignitions; CO_2 and OH do not have any peaks. These results
 216 imply that, rather than the spontaneous auto-ignition like the 0-D ignitions, deflagrations with a
 217 slow propagation speed can play a critical role in consuming the fuels and generating the products.
 218 Local high-temperature mixtures by large T' ignite very rapidly and develop into deflagrations
 219 such that the deflagration mode of combustion prevails over the entire domain, thereby leading to
 220 the temporal spread of HRR. The detailed analysis of localized physicochemical characteristics of
 221 HCCI combustion is an ongoing research topic.

222 As found in previous studies [15–17, 22–24], the deflagration mode of combustion can be domi-
 223 nant for cases with large T' , and hence, the propagation characteristics of each PRF/air deflagration
 224 wave become more important than the chemical kinetics associated with initiating nascent ignition
 225 kernels. Moreover, it is found from 1-D simulations that the laminar flame speeds of PRF/air
 226 mixtures with different octane numbers are nearly identical ($S_L \approx 0.2$ m/s at $p_0 = 40$ atm and
 227 $T_0 = 850$ K). Therefore, it is reasonable to expect that overall combustion is not very different for

different PRF/air mixtures, even though τ_{ig}^0 are widely different, particularly if T' is large enough to induce a sufficient amount of deflagration.

The ignition characteristics of PRF/air mixtures can be further identified by investigating the instantaneous isocontours of HRR for Cases 1–3 approximately at each τ_{ig} as shown in Fig. 5. The HRR, $\dot{q}$, is normalized by the maximum $\dot{q}$ of the corresponding 0-D ignition of the PRF50/air mixture, $\dot{q}_m^0 = 553.7 \text{ J/mm}^3\text{s}$. It is readily observed that for small T' (Case 1), $\dot{q}$ occurs nearly simultaneously over the entire domain as spontaneous ignition. For large T' (Case 3), however, high $\dot{q}$ occurs in thin sheets while low levels of heat release exist in between. This suggests that the mixed mode of spontaneous auto-ignition and deflagration occurs in Case 3, which results in the advancement of the overall combustion, the temporal spread of $\bar{q}$, and the reduction of peak $\bar{q}$.

3.2. Chemical explosive mode analysis

The ignition characteristics of PRF/air mixtures are further identified using the chemical explosive mode analysis (CEMA). CEMA has been developed for systematically detecting critical flame features such as ignition, extinction, and flame fronts and applied to DNSs of lifted flames in heated coflows [45–48], reacting jets in cross-flows [49, 50], and ignition of hydrocarbon fuel/air mixtures under HCCI conditions [22, 24, 51].

CEMA is briefly summarized here and readers are referred to [46] for more details. In general, the local chemical characteristics in chemically reacting flows can thoroughly be accounted for by the Jacobian of the chemical source term, $\mathbf{J}_\omega (\equiv \partial \omega / \partial \mathbf{y})$, in the governing equations, where $\mathbf{y}$ is the solution vector of species concentration and temperature, and ω is the chemical source term. Chemical explosive mode (CEM) is then defined as an eigenmode of $\mathbf{J}_\omega$ where the real part of the eigenvalue, λ_e , is positive [46]. By definition, CEM represents the reciprocal chemical timescale of a local mixture such that a mixture with CEM is destined to explode if it is isolated from any significant loss in heat or radicals. Therefore, CEM can be considered as an intrinsic chemical feature of ignitable mixtures.

To measure the competition between CEMs and the losses, a Damköhler number, Da_c , is adopted, which is defined as:

$$Da_c = \lambda_e \cdot \chi^{-1}, \quad (1)$$

where scalar dissipation rate, $\chi (= 2D|\nabla c|^2)$, represents a reciprocal characteristic timescale of the diffusion or loss term [24, 46–48, 51]. Note that c and D are the progress variable and the thermal

diffusivity of local mixture, respectively. c is defined as $c \equiv Y_c/Y_c^{\text{Eq}}$, where $Y_c = Y_{\text{CO}_2} + Y_{\text{CO}}$, and Y_c^{Eq} is the corresponding equilibrium value of Y_c . A mixture with large positive Da_c will likely lead to actual ignition. However, a mixture with large negative Da_c represents strongly burning flames. Note that $Da_c = 1$ indicates ignition or extinction states of steady state combustion.

Figure 6 shows isocontours of λ_e , Da_c , χ , and temperature for Cases 1 and 3 at each τ_{ig} . To clearly show the reaction fronts, λ_e and Da_c are shown on a logarithmic scale together with the sign of λ_e such that large positive values in Figs. 6a and b represent unburned mixtures while large negative values denote burned mixtures. For both cases, the reaction fronts represented by the thick black lines ($Da_c = 1$) separate the burned and unburned mixtures and correspond to either spontaneous ignition or deflagration. It is readily observed from the figures of Da_c that for Case 1, the reaction fronts delineate the auto-igniting (red) region with large positive Da_c from the post-ignition (blue) region with large negative Da_c . It is also of interest to note that $Da_c \gg O(1)$ upstream of the reaction fronts indicates that the reaction fronts are spontaneous ignition.

For Case 3, however, there exist three distinct regions: an auto-igniting region (red), a post-ignition region (blue), and a deflagration region (green). The green region represents reaction fronts upstream of the auto-igniting region which coincide with strips where χ balances λ_e , a feature of deflagration waves propagating through unburned mixtures prior to the occurrence of auto-ignition. These results also indicate that the reaction fronts of Case 3 are deflagration waves rather than spontaneous ignition fronts.

4. Effect of turbulence

In most previous DNS studies of HCCI combustion [16, 17, 22–24], it was found that turbulence with short τ_t and large u' is more effective at dissipating initial temperature inhomogeneities than that with long τ_t and small u' . Therefore, overall combustion is retarded while occurring by spontaneous ignition. However, it was also found from [23] that turbulence with short τ_t and large u' can advance overall SACI combustion by increasing turbulent flame area. In this section, therefore, the effect of turbulence on the ignition of PRF/air mixtures is elucidated. Four DNSs (Cases 7–10) were performed with greater u' for different PRF/air mixtures (see Table 1 for details of the parameters).

Figure 7 shows the temporal evolution of $\bar{p}$ and $\bar{q}$ for the additional cases with $u' = 2.5$ m/s

and the corresponding cases with $u' = 0.5$ m/s for PRF50 and PRF80. Several points are to be noted from the figure. For cases with T' of 60 K, which is relatively small considering that it induces a small range of ignition delays of the initial mixture, turbulence with short τ_t and large u' can effectively homogenize the mixtures. Therefore, both τ_{ig} and the peak of $\bar{q}$ are increased and overall, combustion is more apt to occur by spontaneous ignition for both PRF/air mixtures. For cases with a larger T' of 120 K, however, τ_{ig} is reduced and the peak value of $\bar{q}$ is increased with increasing u' . This is opposite to the cases with small T' and what was found in previous studies [16, 17, 22–24]. This result is more similar to the ignition characteristics of SACI combustion [23].

4.1. Ignition Damköhler number

To quantify the effect of turbulence on the early ignition characteristics, we introduce an ignition Damköhler number, Da_{ig} , which evaluates the overall competition between ignition and turbulence dissipation during the early phase of HCCI combustion:

$$Da_{ig} = \tau_t / \tau_{ig,10\%}, \quad (2)$$

where τ_t is the turbulence timescale of the initial turbulence and $\tau_{ig,10\%}$ is the lowest 10% ignition delay of the initial mixture, which represents the shortest ignition timescale of the initial mixtures. If $Da_{ig} \gg O(1)$, the occurrence of nascent ignition kernels and their evolution to deflagrations are nearly independent of turbulence. On the contrary, if $Da_{ig} \lesssim O(1)$, ignition is significantly affected by turbulence. Note that if $Da_{ig} \ll O(1)$, the homogenization of the initial mixture by turbulence is finished much earlier than the corresponding 0-D ignition delay and, as such, overall combustion becomes similar to homogeneous 0-D ignition.

For Cases 2 and 7 ($T' = 60$ K), $Da_{ig} = 1.85$ and 0.37 ($\tau_{ig,10\%} \approx 1.35$ ms), respectively and hence, the development of nascent ignition kernels is more disturbed by turbulence in Case 7; the initial mixture is more homogenized by large u' with short τ_t ; consequently, the overall combustion of Case 7 is retarded as shown in Fig 7. For Cases 3 and 8 ($T' = 120$ K), however, $Da_{ig} = 14.5$ and 2.9 ($\tau_{ig,10\%} \approx 0.17$ ms), respectively such that the early phase of ignition becomes nearly independent of turbulence. Once deflagrations are developed from the ignition kernels, their evolutions can be highly affected by local turbulence. For these cases, the turbulent flames exist within the corrugated flamelet and thin reaction zone regimes [52, 53] such that large u' of Case 8 advances the overall combustion by increasing turbulent flame area compared to Case 3. The turbulent flame

regime will further be discussed in the next section. Figure 8 shows the instantaneous isocontours of HRR for Cases 3 ($u' = 0.5$ m/s) and Case 8 ($u' = 2.5$ m/s), which readily identify the increase of turbulent flame area by large u' of Case 8. Note that the above Da_{ig} analysis holds for Cases 7–10 within the range of $0 \sim 20\%$ of τ_{ig} in Da_{ig} .

It is of interest to note that even for the SACI cases of which mean temperature is above the NTC regime (see Cases 4 and 10 in [23]), the ignition Damköhler number analysis can directly be applied. From the results of the two SACI cases, it is readily observed that the corresponding Da_{ig} of the two cases are $\sim O(10)$. As such, large u' of Case 10 results in the advancement of the overall combustion compare to that of Case 4. Note that the high temperature source can be regarded as large T' in the present study.

The occurrence of the early deflagration can be identified by the density-weighted displacement speed, S_d^* , which also shows the propagation characteristics of the combustion waves. S_d^* is defined by [45, 54, 55]:

$$S_d^* = \frac{1}{\rho_u |\nabla Y_k|} \left(\dot{\omega}_k - \frac{\partial}{\partial x_j} (\rho Y_k V_{j,k}) \right), \quad (3)$$

where Y_k , $V_{j,k}$, and $\dot{\omega}_k$ denote the species mass fraction, the species diffusion velocity in the j -direction, and the net production rate of species k , respectively. ρ_u is the density of the unburnt mixture calculated from the local enthalpy and fresh mixture conditions [16, 17, 22–24]. The isocontour of $Y_c = 0.065$ is chosen to evaluate the displacement speed for all cases as in previous studies [22–24]. This particular isocontour coincides approximately with the location of maximum $\dot{q}$ of PRF/air mixtures.

Figure 9 shows the temporal evolutions of the mean front speed, $\overline{S_d^*}$, for the DNS cases, all of which are normalized by the corresponding laminar flame speed, S_L . As in previous studies [22, 23], S_L was estimated from a transient 1-D reactive simulation. The initial species composition, pressure, and temperature for the 1-D simulations were specified the same as those of the mean values in 2-D DNSs without any fluctuations. A high-temperature ignition source was then added on the initial constant temperature field to generate a combustion wave, which emanates from the source, propagating into the reactive mixture ahead of it. Auto-ignition in the reactive mixture does not occur prior to τ_{ig}^0 such that the measured displacement speed, S_d^* , of the combustion wave can be considered as the laminar flame speed, S_L , at the corresponding pressure. S_L is found to be approximately 0.2 m/s for all PRF/air mixtures and remain nearly identical during the combustion

343 wave propagation.

344 As found in previous studies [16, 17, 22–24], the mean front speeds show a characteristic ‘U’
345 shape of HCCI combustion. The initial thermal run-away in the nascent ignition kernel results in
346 large $\overline{S_d^*}$ during the early phase of combustion. In the same way, the simultaneous auto-ignition
347 of the unburned end-gas leads to the sudden increase of $\overline{S_d^*}$ during the final phase of combustion
348 [22–24, 55].

349 It is also observed that after the initial thermal run-away, $\overline{S_d^*}$ similar to S_L develops earlier
350 with increasing T' and the duration of the region with a constant front speed at the bottom of
351 the ‘U’ shape also increases with increasing T' . Note that the start of a relatively-constant front
352 speed implies the occurrence of deflagrations. For the cases with large T' , the start of deflagration
353 mode of combustion coincides regardless of fuel composition and u' , verifying that for cases with
354 $Da_{ig} \gg O(1)$, the role of turbulent mixing on the development of nascent ignition kernels and their
355 evolution into deflagrations is negligible.

356 5. Discussion

357 After the successful development of deflagrations from ignition kernels by large Da_{ig} , the tem-
358 poral evolutions of deflagrations depend highly on their propagation characteristics and local tur-
359 bulence conditions [52]. It is found from the present DNSs that the laminar flame thickness, l_L ,
360 and speed, S_L , are approximately 0.04 mm and 0.2 m/s, respectively. Therefore, for Cases 3 and 6,
361 $l_e/l_L \sim O(10)$ and $u'/S_L \sim O(1)$. For Cases 8 and 10, however, $l_e/l_L \sim O(10)$ and $u'/S_L \sim O(10)$.
362 As such, all turbulent flames with large T' exist within the corrugated flamelet and thin reaction
363 zone regimes in the regime diagram for premixed turbulent combustion [52, 53] as shown in Fig. 10.
364 This implies that large u' induces more corrugated flame structures and thus, enhances the turbu-
365 lent burning rate by increasing turbulent flame area as shown in Fig. 8. Note that for the cases
366 considered in Fig. 10, the occurrence of the ignition kernels and subsequent development of the
367 deflagrations are finished much earlier than one eddy turnover time of turbulence, and hence, u'
368 and l_e are found to be nearly identical to those of the initial conditions such that the locations of
369 the cases on the turbulent combustion regime remain the same.

370 In summary, two key parameters should be considered to understand the effect of turbulence
371 on the characteristics of hydrocarbon-fueled HCCI combustion: Da_{ig} and u'/S_L . If Da_{ig} is large

372 enough to successfully develop deflagrations in HCCI combustion, overall combustion can be ad-
 373 vanced with large u'/S_L since the corresponding turbulent flames exist within the corrugated
 374 flamelet and thin reaction zone regimes. On the contrary, if Da_{ig} is small enough to disturb the
 375 early development of ignition kernels, the overall combustion is retarded because turbulence with
 376 short τ_t and large u' can effectively homogenize the initial mixture fluctuations. It is of great
 377 importance to note that 2-D turbulence is qualitatively different from 3-D turbulence such that
 378 the findings from the present 2-D DNSs need to be verified and generalized by a parametric 3-D
 379 DNS study, which is a future research topic.

380 The analysis of Da_{ig} together with turbulent flame regime can be applied to SACI combustion;
 381 turbulence with large u' can advance the overall SACI combustion exhibiting very large Da_{ig}
 382 ($\gg 1$) by spark ignition as in [23]. In the same way, it may be conjectured that 3-D turbulence in
 383 SACI combustion may also advance the overall combustion more than 2-D turbulence, which was
 384 observed in [25], because the effect of vortex stretching in 3-D turbulence can locally strengthen
 385 u' more than 2-D turbulence, resulting in the increase of turbulent flame area. Due to the same
 386 vortex stretching effect, 3-D turbulence with small Da_{ig} may retard the overall HCCI combustion
 387 more than 2-D turbulence by homogenizing the initial mixture inhomogeneities [19].

388 It is worth mentioning that in addition to the DNS studies of HCCI combustion, there have been
 389 many attempts to develop and validate turbulent combustion models for large eddy simulations
 390 (LES) and Reynolds averaged Navier-Stokes simulations (RANS) based on DNS data. Several
 391 models including flamelet-based models [56], probability density function (PDF) based models [57],
 392 and conditional moment closure (CMC) based model [58] for HCCI combustion have been proposed.
 393 These combustion models show good agreements with DNS results especially for small temperature
 394 and composition stratifications. As such, the present DNS database can be further utilized to
 395 develop turbulent combustion models for HCCI combustion with large thermal stratifications.

396 6. Conclusions

397 The effects of PRF composition, T' , and u' on the ignition of lean PRF/air mixtures at high
 398 pressure and intermediate temperature are investigated by 2-D DNSs with a 116-species reduced
 399 mechanism. The chemical explosive mode and displacement speed analyses verify that, in general,
 400 larger T' induces greater temporal spreading of the mean HRR regardless of PRF composition

because the deflagration mode is predominant at the reaction fronts for large T' . However, spontaneous ignition prevails for small T' and, hence, simultaneous auto-ignition occurs throughout the whole domain, resulting in an excessive HRR. The effect of fuel composition on the ignition of PRF/air mixtures is found to be significantly reduced with increasing T' because the deflagration mode prevails at the reaction fronts and the propagation characteristics of these deflagrations are nearly identical.

The ignition Damköhler number, Da_{ig} , defined by the ratio of turbulence timescale to the shortest ignition delay of initial mixtures, was proposed to evaluate the effects of turbulence on the early evolution of deflagrations from ignition kernels. For cases with $Da_{ig} \lesssim O(1)$, turbulence with large u' can effectively homogenize the mixtures and disturb the evolution of deflagrations from ignition kernels due to the short turbulence timescale compared to the ignition timescale. Therefore, the overall combustion is retarded and more apt to occur by spontaneous ignition. For cases with $Da_{ig} \gg O(1)$, however, the occurrence of nascent ignition kernels and their evolution to deflagrations are not affected by turbulence and the subsequent development of deflagrations occur only within the corrugated flamelet and thin reaction zone regimes of turbulent combustion. As such, turbulence with large u' can advance the overall combustion by increasing turbulent flame area.

Acknowledgements

The work at Ulsan National Institute of Science and Technology was supported by the Basic Science Research Program through the National Research Foundation of Korea funded by the Ministry of Education, Science and Technology (No. 2011-0008201). SOK and MBL were also supported by BK21PLUS funded by the Korea Ministry of Education. The work at Sandia National Laboratories was supported by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences, and Office of Advanced Scientific Computing Research of the US Department of Energy. JHC was also supported as part of the Combustion Energy Frontier Research Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001198. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DEAC04-94AL85000. This research used

resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725 and the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

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A DNS study of ignition of lean PRF/air mixtures with temperature inhomogeneities under high pressure and intermediate temperature

List of Tables

1	Physical and numerical parameters of the DNSs.	19
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List of Figures

1	0-D ignition delays as a function of initial temperature for different PRF/air mixtures at $p_0 = 40$ atm and of $\phi_0 = 0.4$	19
2	Initial temperature (top) and vorticity (bottom) fields of Case 2.	20
3	Temporal evolutions of the mean pressure and mean HRR (left) and the PRR (right) for Cases 1–3 (PRF50; a & c) and Cases 4–6 (PRF80; b & d).	20
4	Temporal evolutions of the mean mass fractions of important species and mean HRR for (a) 0-D case of PRF50/air mixture, (b) Case 1, (c) Case 3, (d) 0-D case of PRF80/air mixture, (e) Case 4, and (f) Case 6.	21
5	Isocontours of the normalized heat release rate for Cases 1–3 (from left to right) at $t/\tau_{ig}^0 = 1.0, 0.94$, and 0.61 , respectively.	21
6	Isocontours of (a) the timescale of the chemical explosive mode, (b) Da_c , (c) temperature, and (d) χ for Case 1 (top) at $t/\tau_{ig}^0 = 1.0$ and Case 3 (bottom) at $t/\tau_{ig}^0 = 0.61$. The solid line denotes the reaction front ($Da_c = 1$).	22
7	Temporal evolutions of the mean pressure and mean HRR for (a) PRF50 and (b) PRF80.	22
8	Isocontours of the normalized heat release rate for Cases 3 (top) and 8 (bottom). From left to right, $t/\tau_{ig}^0 = 0.36$ and 0.52 , respectively.	23
9	Temporal evolution of the mean front speed, $\overline{S_d^*}$, for (a) Cases 2, 3, 7, and 8 (PRF50) and (b) Cases 5, 6, 9, and 10 (PRF80).	23
10	The locations of the cases with small u' (Cases 3 and 6) and large u' (Cases 8 and 10) in the regime diagram for turbulent premixed combustion.	24

Table 1: Physical and numerical parameters of the DNSs.

Case	Fuel	T' (K)	l_e (mm)	u' (m/s)	τ_t (ms)	τ_{ig}^0 (ms)	N
1	PRF50	15	1.25	0.5	2.5	2.5	640
2	PRF50	60	1.25	0.5	2.5	2.5	640
3	PRF50	120	1.25	0.5	2.5	2.5	1280
4	PRF80	15	1.25	0.5	2.5	6.3	640
5	PRF80	60	1.25	0.5	2.5	6.3	640
6	PRF80	120	1.25	0.5	2.5	6.3	1280
7	PRF50	60	1.25	2.5	0.5	2.5	640
8	PRF50	120	1.25	2.5	0.5	2.5	1280
9	PRF80	60	1.25	2.5	0.5	6.3	640
10	PRF80	120	1.25	2.5	0.5	6.3	1280

Figure 1: 0-D ignition delays as a function of initial temperature for different PRF/air mixtures at $p_0 = 40$ atm and of $\phi_0 = 0.4$.

Figure 2: Initial temperature (top) and vorticity (bottom) fields of Case 2.

Figure 3: Temporal evolutions of the mean pressure and mean HRR (left) and the PRR (right) for Cases 1–3 (PRF50; a & c) and Cases 4–6 (PRF80; b & d).

Figure 4: Temporal evolutions of the mean mass fractions of important species and mean HRR for (a) 0-D case of PRF50/air mixture, (b) Case 1, (c) Case 3, (d) 0-D case of PRF80/air mixture, (e) Case 4, and (f) Case 6.

Figure 5: Isocontours of the normalized heat release rate for Cases 1–3 (from left to right) at $t/\tau_{ig}^0 = 1.0, 0.94$, and 0.61 , respectively.

Figure 6: Isocontours of (a) the timescale of the chemical explosive mode, (b) Da_c , (c) temperature, and (d) χ for Case 1 (top) at $t/\tau_{ig}^0 = 1.0$ and Case 3 (bottom) at $t/\tau_{ig}^0 = 0.61$. The solid line denotes the reaction front ($Da_c = 1$).

Figure 7: Temporal evolutions of the mean pressure and mean HRR for (a) PRF50 and (b) PRF80.

Figure 8: Isocontours of the normalized heat release rate for Cases 3 (top) and 8 (bottom). From left to right, $t/\tau_{ig}^0 = 0.36$ and 0.52 , respectively.

Figure 9: Temporal evolution of the mean front speed, $\overline{S_d^*}$, for (a) Cases 2, 3, 7, and 8 (PRF50) and (b) Cases 5, 6, 9, and 10 (PRF80).

Figure 10: The locations of the cases with small u' (Cases 3 and 6) and large u' (Cases 8 and 10) in the regime diagram for turbulent premixed combustion.