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# Effects of initial temperature on autoignition and detonation development in dimethyl ether/air mixtures with temperature gradient

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## Abstract

For large hydrocarbon fuels used in internal combustion engines, different low-temperature and hightemperature chemistries are involved in the autoignition processes under different initial temperatures. As one of the simplest fuels with low-temperature chemistry, dimethyl ether (DME) is considered in this study and one-dimensional autoignitive reaction front propagation induced by temperature gradient is simulated for stoichiometric DME/air mixtures considering detailed chemistry and transport. The emphasis is placed on assessing and interpreting the influence of initial temperature on the detonation development regime. Different initial temperatures below, within and above the negative-temperature coefficient (NTC) region are considered. For each initial temperature, four typical autoignition modes are identified: supersonic autoignitive reaction front (without detonation); detonation development; transonic reaction front; and subsonic reaction front. The detonation development regimes for two fuels, DME and n-heptane, at the same initial temperature and those for the same fuel, DME, at three different initial temperatures respectively below, within and above the NTC region are obtained. Based on these results, the influence of fuel type and initial temperature on detonation development regime are discussed. It is found that the detonation development regime becomes narrower at higher initial temperature. Moreover, the influence of initial temperature on reaction front propagation speed is investigated. The reaction front propagation speed is shown to be strongly affected by different chemistries involved in low and high temperature regions. When only the hightemperature chemistry is involved, the reaction front propagation speed is shown to be less dependent on the initial temperature.

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# 1. Introduction

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Autoignitive reaction front propagation in mixtures with temperature inhomogeneity may occur

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in traditional spark ignition engines (SIEs) and advanced internal combustion engines such as HCCI and SACI engines [1–4]. During such autoignitive reaction front propagation, detonation development happens under certain conditions and it can cause engine knock in SIEs [1,2]. Moreover, such kind of autoignition may cause difficulties in the control of ignition timing in HCCI and SACI engines [3,4]. Therefore, autoignition in mixtures with temperature non-uniformity has received great attention recently (e.g., [5] and references therein).

Zel'dovich [6] first developed the theory on autoignitive reaction front propagation caused by reactivity non-uniformity. It was proposed that different modes of reaction front propagation can be induced by the gradient of ignition delay time and that detonation can develop at certain conditions [6]. The theory of Zel'dovich was verified and extended by many researchers (e.g., [7–11]). Among them, Bradley and coworkers [8,9] investigated different modes of reaction front propagation from a hot spot in syngas/air mixtures using one-dimensional simulation. They studied the critical conditions for detonation development and proposed an operational peninsula within which detonation can develop from temperature inhomogeneity. The detonation peninsula was then used by Bradley and Kalghatgi [2,12,13] in the study of engine knock. It was demonstrated that the detonation peninsula helps to determine the critical conditions for detonation development in engines and thereby it is a very useful tool in the study of engine knock [2,13–16].

Though it was determined only for syngas [8,9], the detonation peninsula was used for different hydrocarbon fuels [2,12,13]. It has not been checked whether this detonation peninsula also works for other fuels besides syngas. Rudloff et al. [14] first suggested the dependence of detonation development regime on fuel and they proposed to conduct simulations for other fuels [8]. Therefore, there is a need to investigate the detonation development regime for fuels other than syngas.

Unlike syngas, large hydrocarbon fuels used in engines usually have complicated low-temperature chemistry and negative-temperature coefficient (NTC) phenomenon. Therefore, at different initial temperatures below, within and above the NTC region, the detonation development regime and autoignitive reaction front propagation behavior may be different. In the literature, direct numerical simulations of autoignition in mixtures with thermal stratification were conducted for several fuels with low-temperature chemistry, e.g., dimethyl ether (DME) [17], n-heptane [18] and iso-octane [4,19]. However, in these studies detonation development was not investigated. Zhang et al. [20] examined the coupling effects of concentration and temperature gradients on autoignition modes and proposed a general critical boundary to separate the spontaneous ignition mode from detonation modes

in the two dimensional concentration and temperature gradient phase space. In our recent work [21,22], the temperature gradient-induced autoignitive reaction front propagation in n-heptane/air mixture was investigated. It was found that the low-temperature chemistry results in complicated reaction-pressure wave interactions. Therefore, it is of interest to further study how the initial temperature affects detonation development regime and autoignitive reaction front propagation for fuels with low-temperature chemistry. Since DME is one of the simplest fuels with low-temperature chemistry, it is studied in the present work.

Based on the above considerations, the objectives of this study are to obtain the detonation development regimes for fuels other than syngas and to examine the effects of initial temperature on autoignitive reaction front propagation and detonation development regime. Unlike our previous studies [21,22] which mainly considered planar geometry, this study focuses on spherical geometry (same as that of Bradley and coworkers [9] and similar to hot/cold spots in engines). Therefore, the detonation development regimes obtained here can be compared with that in [9] for syngas. Furthermore, for the same fuel, DME, the detonation development regimes at different initial temperatures below, within and above the NTC region are obtained and compared in this study.

#### 2. Numerical model and specifications

The present model is the same as that of Bradley and coworkers [9]. We consider the autoignitive reaction front propagation from a hot or cold spot at the center of a closed spherical chamber. The initial temperature distribution is

$$T(t = 0, r) = \begin{cases} T_0 + (r - r_0) \frac{dT_0}{dr} & \text{for } 0 \le r \le r_0 \\ T_0 & \text{for } r_0 \le r \le R_W \end{cases}$$
(1)

where *t* and *r* are respectively the temporal and spatial coordinates;  $r_0$  is the size of hot/cold spot;  $R_W = 10$  cm is the radius of the spherical chamber;  $dT_0/dr$  is the temperature gradient to be specified  $(dT_0/dr < 0$  for hot spot and  $dT_0/dr > 0$  for cold spot); and  $T_0$  is the initial temperature of the mixture outside of the hot/cold spot. The whole computational domain is initially filled with static fuel/air mixture at the pressure of  $P_0 = 40$  atm. We limit our focus to laminar combustion and thereby the initial flow is static without turbulence. At both boundaries (i.e., r = 0 and  $r = R_W$ ), zero flow speed and zero gradients of temperature and mass fractions are enforced.

The transient autoignition process is simulated using the in-house code A-SURF. The conservation equations for one-dimensional, compressible,



Fig. 1. Change of (a) ignition delay time and (b) critical temperature gradient with the initial temperature for stoichiometric DME/air mixture at  $P_0 = 40$  atm.

multi-component, reactive flow are solved in A-SURF using the finite volume method. A-SURF has been successfully used in previous studies on flame propagation, end-gas autoignition and detonation development (e.g., [22–26,32]). The details on governing equations, numerical methods, and code validation for A-SURF can be found in Refs. [22-24] and are presented in the Supplementary Document. In simulation, dynamically adaptive mesh refinement algorithm is used to efficiently and accurately resolve the reaction front, pressure wave, shock wave and detonation. The finest mesh size is  $2 \,\mu m$  and the corresponding time step is 0.4 ns. Numerical convergence has been checked and ensured by further decreasing the time step and mesh size in simulation.

We mainly focus on detonation development regimes for stoichiometric DME/air at different initial temperatures below, within and above the NTC region. Another fuel, n-heptane, is also considered so that detonation development regimes for different fuels can be compared. In simulation, the chemical mechanisms for DME [27] and n-heptane [28] are used. Both mechanisms have been demonstrated to be able to accurately predict ignition (including the NTC behavior) and flame propagation at a broad range of temperature and pressure [27,28].

#### 3. Results and discussion

Figure 1(a) shows the change of ignition delay time,  $\tau_{ig}$ , with the initial temperature,  $T_0$ , for stoichiometric DME/air at  $P_0 = 40$  atm. It is seen that the temperature range of  $872 \text{ K} \le T_0 \le 1010 \text{ K}$  corresponds to the NTC region in which  $\tau_{ig}$  increases monotonically with  $T_0$ . To compare the detonation development regime and autoignitive reaction front propagation under different temperature, three initial temperatures,  $T_0 = 802$  K, 982 K and 1035 K, corresponding to the same ignition delay time ( $\tau_{ig} = 381 \,\mu s$ ) are selected in the following 1D simulations. As shown in Fig. 1(a), these three temperatures are respectively below, within and above the NTC region. For  $T_0$  below the NTC region, low-temperature chemistry plays an important role in the autoignition process and two-stage ignition occurs (see Fig. S9 in the Supplementary Document). With the increase of  $T_0$ , the first-stage ignition caused by low-temperature chemistry is gradually suppressed and eventually single-stage ignition occurs.

According to the reactivity gradient theory of Zel'dovich [6], different modes of reaction front propagation can be observed depending on the magnitude of temperature gradient. Theoretically, the reaction front propagation speed caused by the linear temperature distribution is [6,9]:

$$u_a = \left(\frac{d\tau_{ig}}{dr}\right)^{-1} = \left(\frac{d\tau_{ig}}{dT_0} \cdot \frac{dT_0}{dr}\right)^{-1}$$
(2)

When the reaction front speed  $u_a$  is close to the local sound speed, a, chemical reaction and pressure wave can be coherently coupled to form a developing detonation [6,9]. According to Eq. (2), the critical temperature gradient determined by the condition of  $u_a = a$  is

$$\left(\frac{dT_0}{dr}\right)_c = \left(a\frac{d\tau_{ig}}{dT_0}\right)^{-1} \tag{3}$$

Figure 1(b) shows the critical temperature gradient as a function of initial temperature. Two singular points exist at the boundaries of the NTC region. Within the NTC region, the critical temperature gradient is positive and thereby autoignitive reaction front is initiated from a cold spot (i.e.,  $dT_0/dr > 0$  in Eq. (1)). Below and above the NTC region, the critical temperature gradient becomes negative and thus autoignitive reaction front is initiated from a hot spot (i.e.,  $dT_0/dr < 0$  in Eq. (1)). Similar results have been obtained for n-heptane (see Fig. 1 in Ref. [21]).

Based on the critical temperature gradient, the non-dimensional temperature gradient is defined as [9]:

$$\xi = \frac{dT_0}{dr} / \left(\frac{dT_0}{dr}\right)_c = \frac{a}{u_a} \tag{4}$$

in which the second equation is obtained by using Eqs. (2) and (3).

To quantify the detonation development regime, two non-dimensional parameters have been used by Bradley and coworkers [9]: one is the normalized temperature gradient,  $\xi$ , which represents the ratio between local sound speed and reaction front propagation speed according to Eq. (4); and the other is the non-dimensional time,  $\varepsilon$ , which is the ratio of



Fig. 2. Different autoignition modes (blue square: supersonic autoignitive reaction front; black circle: detonation development; red diamond: subsonic reaction front; green triangle: transonic reaction front) and detonation development regime (within the C-shaped pink curve) for stoichiometric DME/air mixture at  $T_0 = 982$  K and  $P_0 = 40$  atm. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

acoustic time  $(r_0/a)$  to excitation time  $\tau_e$  (defined as the time interval between 5% and maximum heat release rate), i.e.,  $\varepsilon = r_0/(a\tau_e)$ . In simulation, different hot/cold spot sizes,  $r_0 = 2$ , 5 and 8 mm, are considered so that different values of  $\varepsilon$  can be reached.

Figure 2 summarizes the autoignition modes in the plot of  $\xi$  versus  $\varepsilon$  for stoichiometric DME/air mixture at  $T_0 = 982$  K and  $P_0 = 40$  atm. The initial temperature is within the NTC region and thereby a cold spot (i.e.,  $dT_0/dr > 0$  in Eq. (1)) is used to initialize the autoignitive reaction front propagation. As shown in Fig. 2, four typical autoignitive reaction front (without detonation); (2) detonation development; (3) transonic reaction front; and (4) subsonic reaction front. The distributions of temperature, pressure and heat release rate for these four modes are shown in Section 4 in the Supplementary Document.

Figure 2 indicates that detonation development only occurs at certain values of  $\xi$  and  $\varepsilon$ . The detonation development regime is depicted by the C-shaped curve, which is bounded by the lower and upper limits denoted by  $\xi_l$  and  $\xi_u$ , respectively. The temperature gradient-induced detonation develops only for  $\xi_l < \xi < \xi_u$ . At small values of  $\xi$  below the lower branch of the C-shaped curve (i.e.,  $\xi < \xi_l$ ), the reaction front propagation speed is much larger than the local sound speed. Therefore, local chemical reaction and pressure wave cannot be coherently coupled and no detonation is developed. This corresponds to the mode of supersonic autoignitive reaction front (blue squares in Fig. 2). On the contrary, at large values of  $\xi$ above the upper branch of the C-shaped curve

(i.e.,  $\xi > \xi_u$ ), the reaction front propagation speed is smaller than the local sound speed until thermal explosion occurs throughout the unburned mixture. Consequently, there is no detonation development either and this corresponds to the mode of subsonic reaction front (red diamonds in Fig. 2). At small values of  $\varepsilon$  on the left side of the C-shaped curve, the cold spot size is small  $(r_0 = 2 \text{ mm})$  and thus there is not enough time for coupling and mutual reinforcement between chemical reaction and pressure wave even though the reaction front propagates at a speed close to that of sound. Consequently, as shown in Fig. 2, detonation cannot be developed (for  $r_0 = 2 \text{ mm}$  or small value of  $\varepsilon$ ) and this autoignition mode within the transition zone between supersonic autoignitive reaction front and subsonic reaction front is referred to as the mode of transonic reaction front (green triangles in Fig. 2) since its propagation speed of reaction front is close to local sound speed.

Similar modes of autoignitive reaction front propagation have been observed for syngas [9] and n-heptane [21]. Besides, Fig. 2 only shows the results for the initial temperature of  $T_0 = 982$  K within the NTC region. Similar results for  $T_0 = 802$  K and  $T_0 = 1035$  K respectively below and above the NTC region are presented in Fig. S6 of the Supplementary Document. Therefore, four modes of autoignitive reaction front propagation are observed for all the initial temperatures below, within and above the NTC region for stoichiometric DME/air mixture. In addition, the comparison between the autoignition processes within and below the NTC regime (see Section 4 of the Supplementary Document) indicates that both cold and hot spots can induce different autoignition modes.

Figure 3 compares the detonation development regimes of stoichiometric DME/air mixture at three different initial temperatures, which are respectively below, within and above the NTC region (see Fig. 1). For each initial temperature, detonation develops on the right side of the corresponding C-shaped curve. It is seen that the shape of these detonation development regimes is similar, indicating that the non-dimensional parameters  $\xi$  and  $\varepsilon$ can be used to quantify the tendency of detonation development induced by temperature gradient. However, quantitative difference among these detonation development regimes for different initial temperatures is readily observed in Fig. 3. Specifically, the detonation development regime becomes narrower as the initial temperature increases. At fixed value pressure of  $P_0 = 40$  atm, the volumetric energy density (which is equal to the total amount of chemical heat release per unit volume during the constant-volume homogenous ignition) decreases when the initial temperature increases. For the initial temperature of  $T_0 = 802$  K, 982 K and 1035 K, the corresponding volumetric energy density is 9.4 MJ/m<sup>3</sup>, 7.8 MJ/m<sup>3</sup> and 7.4 MJ/m<sup>3</sup>, respectively.



Fig. 3. Detonation development regimes of stoichiometric DME/air mixture at  $P_0 = 40$  am and different initial temperatures. The results for stoichiometric n-heptane/air at  $P_0 = 40$  atm and  $T_0 = 802$  K are also shown. Detonation develops on the right side of the C-shaped curves. At point A,  $\varepsilon = 10$  and  $\xi = 5$ ; and at point B,  $\varepsilon = 15$  and  $\xi = 4$ .

Therefore, with the increase of initial temperature, less amount of heat is released during the coupling and mutual reinforcement between chemical reaction and pressure wave. Consequently, the tendency of detonation development becomes smaller as the initial temperature increases. It is noted that similar dependency of detonation regime on initial temperature has been recently observed for concentrationgradient inducted autoignition modes [30].

Besides, Fig. 3 also shows the detonation development regime for stoichiometric n-heptane/air at  $T_0 = 802$  K and  $P_0 = 40$  atm. It is observed that the detonation development regimes for DME and n-heptane at the same initial temperature and pressure  $(T_0 = 802 \text{ K} \text{ and } P_0 = 40 \text{ atm})$  are not exactly the same. These regimes for DME and n-heptane are both narrower than that for syngas reported by Bradley and coworkers [9,12] (see Fig. 1 in [12]). While the lower limits for detonation development regimes of these three fuels are similar, the upper limit for syngas (CO: $H_2 = 1:1$ , see Fig. 1 in [12]) suddenly increases to around  $\xi = 40$  when  $\varepsilon > 10$  while it stays around or below  $\xi = 10$  for DME and n-heptane (see Fig. 3). Although Rudloff et al. [14] shifted the peninsula of syngas [9,12] along  $\varepsilon$ -axis considering the large uncertainty in the computation of  $\tau_e$ , there are still significant discrepancies among the upper limits for detonation development in syngas, n-heptane and DME. Therefore, detonation development regime depends on fuel (the reason for such kind of fuel dependency is not clear and deserves further study). To achieve quantitative prediction of engine knock, we need use the detonation development regime for specific fuel rather than that for syngas.

Figure 4 shows the autoignition processes for different initial temperatures,  $T_0 = 802$  K, 982 K



Fig. 4. Temporal evolution of (a) temperature and (b) pressure distributions for stoichiometric DME/air at different initial temperatures but the same value of  $\varepsilon = 10$  and  $\xi = 5$  (point A in Fig. 3).



Fig. 5. Change of reaction front propagation speed,  $S/D_{CJ}$ , with its location,  $R_f/r_0$ , for stoichiometric DME/air at different initial temperatures but the same value of  $\varepsilon = 10$  and  $\xi = 5$  (point A in Fig. 4). The sound speeds at  $T_0 = 802$  K and 1035 K and CJ detonation speed ( $D_{CJ}$ ) are depicted by the horizontal dashed lines.

and 1035 K. The initial temperature distributions and hot/cold spot sizes (shown in Fig. S7 in the Supplementary Document) for these three cases are specified so that they correspond to nearly the same value of  $\varepsilon = 10$  and  $\xi = 5$  (point A in Fig. 3). Figure 4 shows that detonation develops only for  $T_0 = 802$  K and  $T_0 = 982$  K. For  $T_0 = 802$  K, a foregoing shock is first formed in front of the reaction front (see the line corresponding to  $t = 352.4 \,\mu$ s). Then local thermal explosion occurs between the reaction front and shock wave, which results in the development of an over-driven detonation. Similar observation has been obtained in our previous study (see Fig. 4 in Ref. [21]). When the initial temperature is increased from  $T_0 = 802$  K to  $T_0 = 982 \text{ K}$ , the denotation development appears later as shown in Fig. 4. This is due to the facts that only single-stage ignition happens at  $T_0 = 982 \text{ K}$ while two-stage ignition happens at  $T_0 = 802 \text{ K}$ (shown by Fig. S9 in the Supplementary Document), and that at  $T_0 = 802$  K the low-temperature chemical heat release during the first stage ignition promotes the denotation development [22]. Besides, Fig. 4(b) shows that the maximum pressure for  $T_0 = 802 \text{ K}$  is much higher than that for  $T_0 = 982$  K. This is also because the volumetric energy density decreases as the initial temperature increases. For  $T_0 = 1035$  K, Fig. 4 shows that thermal explosion occurs throughout the unburned mixture around  $t = 384 \,\mu s$  and there is no detonation development. It is consistent with Fig. 3 which indicates that this case corresponds to the mode of subsonic reaction front propagation since point A is located above the upper branch of the C-shaped curve for  $T_0 = 1035 \text{ K}.$ 

Figure 5 depicts the corresponding reaction front propagation speed for these three cases shown

in Fig. 4. For  $T_0 = 802$  K, the reaction front is first supersonic and it evolves into a denotation propagating at the Chapman-Jouguet (CJ) detonation speed,  $D_{CJ} = 1860$  m/s. It is noted that the CJ detonation speed is not sensitive to the change of initial temperature. With the increase of initial temperature, the reaction front propagation speed at the beginning with  $R_f/r_0 < 1.0$  decreases and it becomes subsonic for  $T_0 = 982$  K and  $T_0 = 1035$  K. For  $T_0 = 1035$  K, the reaction front propagation speed increases abruptly when it is located around  $R_f/r_0 = 1$  and its speed can be above  $10^4$  m/s due to the thermal explosion occurring throughout the unburned mixture. It is noted that for these three initial temperatures, we have nearly the same value of  $\xi = 5$ . According to Eq. (4), the reaction front propagation speed should have close value of  $u_a = a/\xi = a/5$ . However, the numerical results in Fig. 5 indicate that there exists great discrepancy among speeds for different initial temperatures. This is because the theoretical results in Eq. (4) are based on the initial temperature distribution, which changes during the autoignition process [9,21] (Such change may limit the validity of the obtained peninsula diagram. Nevertheless, as pointed out by one of the reviewers, Robert et al. [16] proposed a local criterion for the existence of a developing detonation on the base of the peninsula diagram in [8,9]. This criterion was validated by 3D Large Eddy Simulation of knock and superknock resolving explicitly the coupling of the reaction and pressure wave in combustion chamber of a SIE [16]. The work of Robert et al. [16] seems to confirm the legitimacy of the peninsula diagram in [8,9], despite of its theoretical limitations). During the autoignition process, different chemistries are involved for different initial temperatures below, within and above the NTC region. Therefore, at the same value of  $\varepsilon = 10$  and  $\xi = 5$ , the reaction front propagation speed is greatly affected by initial temperature as shown in Fig. 5.

To exclude the influence of chemistry, we choose different initial temperatures of  $T_0 = 1035 \text{ K}$ , 1100 K, 1150 K and 1200 K all above the NTC region so that only high-temperature chemistry is involved. The initial temperature distributions and hot spot sizes (shown in Fig. S8 in the Supplementary Document) for these processes are specified so that they correspond to nearly the same value of  $\varepsilon = 15$  and  $\xi = 4$  (point B in Fig. 3). As expected, the tendency of detonation development decreases when the initial temperature increases. This is demonstrated by Fig. 6, which shows that detonation develops for  $T_0 = 1035$  K, but not for  $T_0 = 1200 \text{ K}$ . Since only the high-temperature chemistry is involved and the values of  $\varepsilon$  and  $\xi$ are the same for both initial temperatures, the only difference is the volumetric energy density  $(7.4 \text{ MJ/m}^3 \text{ for } T_0 = 1035 \text{ K} \text{ and } 6.4 \text{ MJ/m}^3 \text{ for}$  $T_0 = 1200$  K). This indicates that besides  $\xi$  and  $\varepsilon$ , a third parameter related to the initial temperature



Fig. 6. Temporal evolution of (a) temperature and (b) pressure distribution for stoichiometric DME/air at  $T_0 = 1035$  K and  $T_0 = 1200$  K and the same value of  $\varepsilon = 15$  and  $\xi = 4$  (point B in Fig. 3).

or volumetric energy density is needed to quantify the detonation development condition. It is consistent with the idea in Ref. [14] which introduced a third parameter,  $\pi$  (obtained via experiments), to evaluate the chemical energy left in the end gases and to access the impact of auto-ignition events on the pressure variation. In addition, Robert et al. [29] and Yu et al. [31] found that knock intensity in SIEs is directly proportional to the fresh gases mass burned by auto-ignition. Therefore, an efficient way to quantify the amplification of pressure wave fed by the energy available in the mixture is crucial to predict detonation development.



Fig. 7. Change of reaction front propagation speed,  $S/D_{\rm CJ}$ , with its location,  $R_f/r_0$ , for stoichiometric DME/air at different initial temperatures but the same value of  $\varepsilon = 15$  and  $\xi = 4$  (point B in Fig. 4). The sound speeds at  $T_0 = 1035$  K and 1200 K and CJ detonation speed ( $D_{\rm CJ}$ ) are depicted by the horizontal dashed lines.

Figure 7 shows the reaction front propagation speeds for four different initial temperatures but the same value of  $\varepsilon = 15$  and  $\xi = 4$ . It is seen that the propagation speeds are relatively close to each other compared to those shown in Fig. 5. For all the cases in Fig. 7, only the high-temperature chemistry is involved; while for cases in Fig. 5, different lowtemperature and high-temperature chemistries are involved. Therefore, this further demonstrates that the reaction front propagation speed is affected by chemistry.

# 4. Conclusions

One-dimensional autoignitive reaction front propagation induced by temperature gradient is simulated for stoichiometric DME/air mixtures considering detailed chemistry and transport. The autoignitive reaction front propagation and detonation development regimes at three initial temperatures respectively below, within and above the NTC region are investigated. For each initial temperature, four typical autoignition modes are identified: (1) supersonic autoignitive reaction front (without detonation); (2) detonation development; (3) transonic reaction front; and (4) subsonic reaction front. The detonation development regime caused by temperature gradient can be identified in the plot of two non-dimensional parameters, namely the normalized temperature gradient,  $\xi$ , and the ratio of acoustic time to excitation time,  $\varepsilon$ . At different initial temperatures, the detonation development regimes in the  $\xi - \varepsilon$  plot are shown to be qualitatively similar but quantitative difference is observed. With the increase of initial temperature, the detonation development regime becomes narrower since the volumetric energy density of the mixture becomes smaller. Moreover, it is found that the detonation development regimes for DME and n-heptane at the same initial temperature and pressure are not exactly the same. Therefore, the detonation development regime does depend on fuel. During the autoignition process, different chemistries are involved for different initial temperatures below, within and above the NTC region. Therefore, at the same value of  $\varepsilon$  and  $\xi$ , the reaction front propagation speed is shown to be affected by initial temperature. When the initial temperature is above the NTC region so that only high-temperature chemistry is involved, the reaction front propagation speed is shown to be less dependent on initial temperature.

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#### Supplementary materials

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