

Reaction front propagation initiated by a hot spot in premixed n-heptane/air mixture at low temperature

Peng Dai, Zheng Chen

SKLTCS, Department of Mechanics and Engineering Science, College of Engineering,
Peking University, Beijing 100871, China

1 Introduction

Engine knock has received increasing attention recently [1, 2], especially considering its constraint on engine downsizing and gasoline direct injection [3, 4]. It is generally accepted that knocking in spark ignition engine (SIE) might be caused by end-gas autoignition [5]. Therefore, understanding autoignition mode and reaction-pressure wave interaction are helpful to reveal knock mechanism [6]. Zel'dovich [7] first theoretically analyzed the interaction between autoignition front and pressure wave as well as different autoignition modes in the presence of non-uniform reactivity. In the following decades, many theoretical [8, 9] and numerical [10-14] studies were conducted to further assess the effects of reaction and pressure wave interaction on reaction front propagation. The hot spot model with linear temperature distribution was popularly used in these studies as initial condition.

However, previous studies were mainly focused on simplified reaction models or simple fuels such as H_2 , CO and CH_4 . For example, Gu et al. [11] demonstrated that different propagation modes of autoignition front can be initiated by temperature gradient in syngas/air mixture and they found a detonation peninsular in the plot of two non-dimensional parameters, namely the normalized temperature gradient and the ratio of acoustic time to excitation time. The detonation peninsular was used for large hydrocarbon fuels even though it was obtained from simulation for syngas [15].

Only a few studies considered large hydrocarbon fuels with low-temperature chemistry which leads to negative-temperature coefficient (NTC) phenomenon [16, 17]. El-Asrag et al. [18] observed three ignition stages for DME/air mixture in NTC regime for both 0D (homogeneous) and 2D direct numerical simulation. They discussed the effects of NO_x addition on these ignition stages. Ju et al. [19] investigated the ignition and flame propagation initiated by a hot kernel in n-heptane/air mixture at both low and high temperatures. It was found that there are two flame structures respectively dominated by high- and low-temperature chemistries. Yoo and coworkers [20, 21] examined the effects of turbulence on autoignition. However, in these studies, shock and detonation caused by the interaction between chemical reaction and pressure wave were not investigated.

Recently, we have studied different autoignition modes of n-heptane/air mixture caused by a cool spot with positive temperature gradient [14]. It was found that shock compression of the mixture in front of the deflagration wave produces an additional ignition kernel, which determines the autoignition modes. Only planar configuration was considered in our previous study [14]. As an extension of [14], here we also consider a spherical configuration since autoignition occurs at hot spot in practical engines. Moreover, unlike [14] here emphasis is focused on hot-spot induced autoignition modes in temperature below the NTC regime, at which multi-stage ignition of n-heptane occurs.

The objective of the present study is to investigate the interaction among different ignition stages of n-heptane and pressure waves generated by a hot spot with negative temperature gradient. First, different ignition stages in homogeneous n-heptane/air mixture will be identified. Then, different autoignition modes in 1D planar and spherical configurations will be discussed. It will be shown that different pressure waves generated by different ignition stages determine the autoignition mode.

2 Model and specifications

In order to investigate the interaction among different ignition stages and pressure waves during reaction front propagation, transient ignition processes initiated by a hot spot in 1D, adiabatic, planar or spherical chamber are simulated (see Fig. 1). Figure 1 (c) shows the initial temperature distribution in planar geometry. The temperature is linearly distributed within the hot spot ($0 \leq x \leq 5$ mm) with a negative gradient and a mean value of 780 K while it is uniform everywhere outside the hot spot. Stoichiometric n-heptane/air initially at 40 atm is considered here. For spherical configuration, the initial condition is similar to that in Fig. 1 (c): the radius of the hot spot is $r_0 = 5$ mm and the temperature at $r_0/2$ is 780 K. The length or radius of the computation domain is 10 cm and adiabatic and reflective boundary conditions are adopted for both sides. The 1D ignition process is simulated using the in-house code A-SURF which uses a multi-level, dynamically adaptive mesh refinement algorithm to maintain adequate numerical resolution of the flame, compression wave, shock wave, and detonation. The details on the governing equations, numerical schemes, and code validation can be found in [22, 23]. It has been demonstrated in our previous studies [14, 24] that A-SURF can accurately resolve flame, shock wave and detonation wave.

The skeletal mechanism for n-heptane oxidation [25] is used in simulation. This mechanism has been demonstrated to be able to accurately predict ignition (including NTC regime) and flame propagation of n-heptane/air mixtures at a broad range of temperatures and pressures [25].

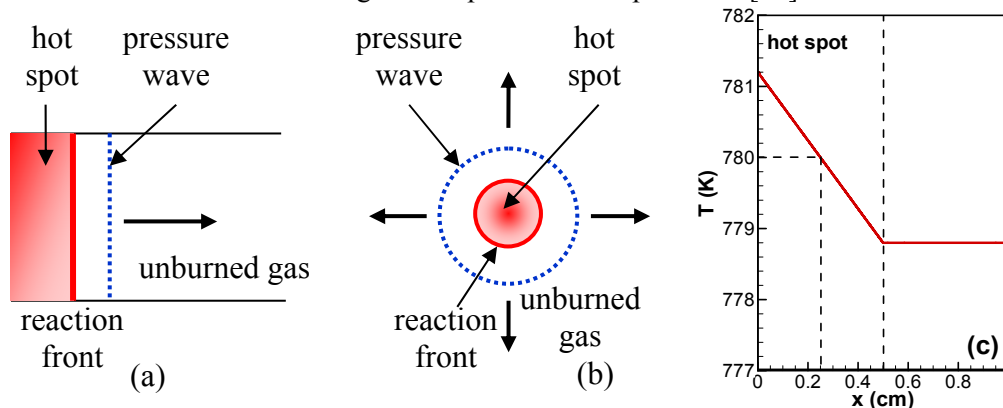


Fig. 1 Schematic plot of 1D (a) planar and (b) spherical configuration for autoignition front propagation initiated by a hot spot. The initial temperature distribution in a planar geometry is shown in (c).

3 Results and Discussion

For large hydrocarbon fuels, the ignition process is usually dominated by different chemical paths at different temperature ranges, and multiple ignition stages during the entire ignition process at low temperatures [16–18]. Figure 2 shows homogeneous (0D) ignition processes as well as the local ignition process initially at $x = 8$ cm in 1D planar geometry with a hot spot (see Fig. 4). Three ignition stages with different heat release peaks and temperature increments are observed. Similar three-stage ignition process was also observed by El-Asrag et al. [18] for DME/air mixture. These three ignition stages are respectively dominated by low-, intermediate- and high-temperature chemistries [16, 18]. Therefore, we call them low-temperature ignition (LTI), intermediate-temperature ignition (ITI), and high-temperature ignition (HTI), respectively.

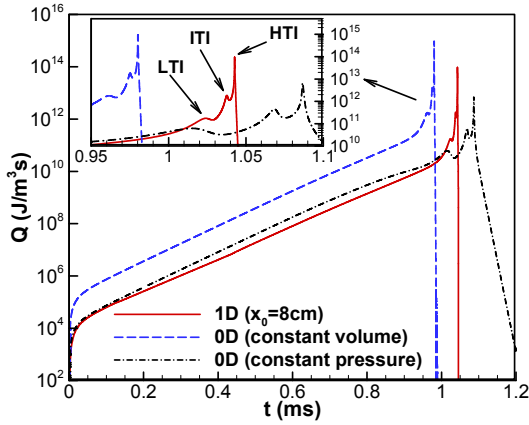


Fig. 2 Temporal evolution of heat release rate in homogeneous (0D) systems as well as at $x_0=8$ cm in 1D planar system for stoichiometric n-heptane/air mixture. The initial pressure and temperature are respectively $P_0=40$ atm and $T_0=778.8$ K.

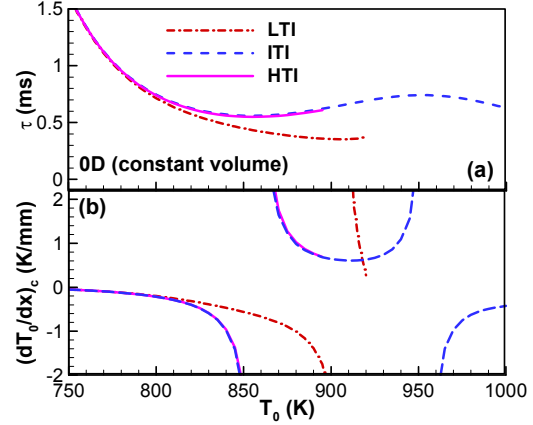


Fig. 3 (a) Ignition delay time and (b) critical temperature gradient for different ignition stages (LTI, ITI, and HTI) as a function of initial temperature for stoichiometric n-heptane/air mixture at $P_0=40$ atm.

In order to investigate the possible interaction among these ignition stages and pressure waves generated by initial temperature gradient, the ignition delay times of LTI, ITI and HTI (defined based on the maximum heat release rate, see Fig. 2) in constant-volume homogeneous ignition are plotted in Fig. 3 (a). It is noticed that the ignition delay time of HTI is actually the global ignition delay time for the entire ignition process. According to Fig. 3(a), the NTC regime is $850 \leq T_0 \leq 960$ K. In absence of heat conduction and mass diffusion, there exists a specific value of temperature gradient at which autoignition front propagates at the speed of sound, which is called critical temperature gradient [7, 11]:

$$\left(\frac{dT_0}{dx}\right)_c = a^{-1} \left(\frac{d\tau}{dT_0}\right)^{-1} \quad \text{or} \quad \left(\frac{dT_0}{dr}\right)_c = a^{-1} \left(\frac{d\tau}{dT_0}\right)^{-1} \quad (1)$$

where τ and a are respectively ignition delay time and sound speed. Based on the critical temperature gradient, the non-dimensional temperature gradient within the hot spot is introduced [11]:

$$\xi = \frac{dT_0}{dx} \bigg/ \left(\frac{dT_0}{dx}\right)_c \quad \text{or} \quad \xi = \frac{dT_0}{dr} \bigg/ \left(\frac{dT_0}{dr}\right)_c \quad (2)$$

Figure 3 (b) plots the critical temperature gradient for three ignition stages. It is observed that the critical temperature gradient for LTI is different from those for ITI and HTI when $T_0 > 820$ K. However, the critical temperature gradients for different ignition stages are shown to be close to each other when the temperature is low ($T_0 \leq 820$ K). This indicates that at a proper temperature gradient (not necessarily critical temperature gradient, see [11, 14]), all the three ignition stages may couple with pressure waves and thus generate strong chemical-acoustic waves.

Figure 4 shows a typical case manifesting this complex interaction. It is observed in Fig. 4 (a) and (c) that initially the autoignition of the hot spot generates the first detonation wave (D1) as well as a pressure wave in front of it which both propagate towards the right. By examining chemical reactions and state parameters of particles at different initial locations, it is found that the first detonation wave D1 is produced and maintained by the intense high-temperature ignition while the pressure wave ahead is generated by the intermediate-temperature ignition within the hot spot. After the coupling and mutual reinforcement between ITI and the pressure wave, the latter eventually evolves into a shock wave. This pressure wave as well as the subsequent shock wave is called as ITI pressure wave (see Fig. 4d). On the other hand, it is seen in Fig. 4 (d) that there is another weaker pressure wave ahead of the ITI pressure wave. This pressure wave is caused by the low-temperature ignition within the hot spot. It is therefore called as LTI pressure wave. These two pressure waves compress reactants during propagation. At $t=1039 \mu\text{s}$ (line #6 in Fig. 4), the mixture between the ITI pressure wave and detonation

wave D1 autoignites due to compression and finally evolves into the second detonation wave (D2). The first detonation wave (D1) soon degenerates into the shock wave (S1) due to the depletion of the reactants ahead of it. Later, the mixture in front of the second detonation wave D2 autoignites due to the compression of the LTI pressure wave and generates two supersonic autoignition fronts propagating in opposite directions. The second detonation wave D2 becomes the shock wave (S2) when it encounters the supersonic autoignition front propagating to the left.

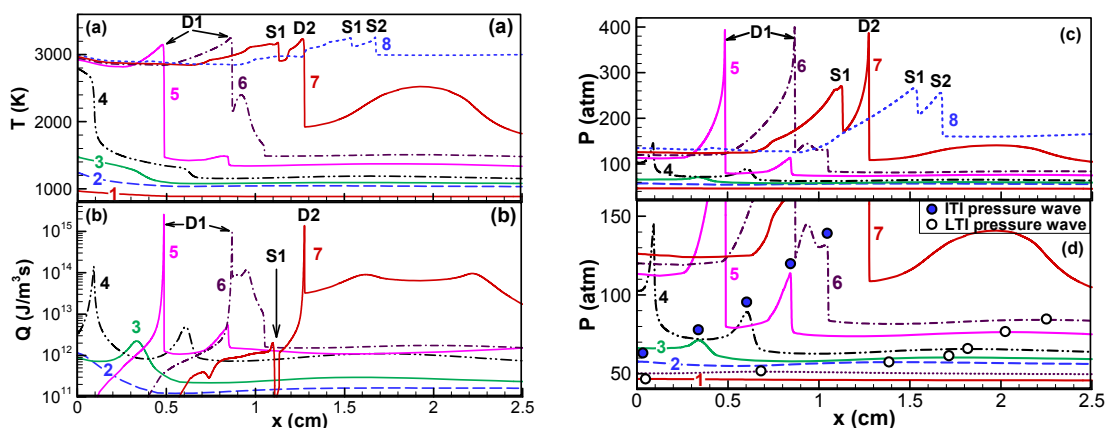


Fig. 4 Temporal evolution of (a) temperature, (b) heat release rate (c) pressure and (d) pressure in enlarged version in planar geometry for $T_0=900$ K, $x_0=5$ mm, and $\zeta=4$. The time sequence is 1: 1000 μ s, 2: 1025 μ s, 3: 1030 μ s, 4: 1034 μ s, 5: 1037 μ s, 6: 1039 μ s, 7: 1041 μ s, 8: 1044 μ s.

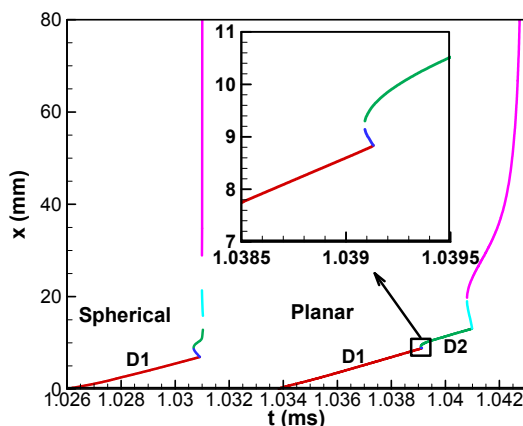


Fig. 5 The change of the location of reaction fronts with time. Lines of different colors represent different reaction fronts: the red denotes the original reaction front; the blue and green ones respectively denote leftward and rightward propagating reaction fronts caused by the first autoignition in the unburned mixture; the cyan and pink ones respectively denote leftward and rightward propagating reaction fronts caused by the second autoignition in the unburned mixture.

It is noted that the above interesting wave phenomenon is a consequence of interaction among different complex chemistries of large hydrocarbon fuel and pressure waves in the presence of temperature gradient. It does not happen for simple fuels or large hydrocarbon fuels at high temperature since there is no multi-stage ignition. In addition, the autoignition process in spherical geometry with the same temperature gradient is similar to that in planar geometry (Fig. 4), except that the ITI pressure wave does not develop to a shock wave and that the autoignition caused by it does not form a detonation. The details are not presented here due to space limitation and will be presented at oral presentation. Figure 5 shows the location of the reaction fronts (lines of different colors represent different reaction fronts) for both planar and spherical geometries. The reaction front is defined as the

location where the local temperature equals to 2000 K. It is seen that for both geometries, autoignition in front of propagating reaction front (detonation or deflagration wave) occurs twice due to the presence of ITI and LTI pressure waves.

4 Conclusions

The ignition and reaction front propagation process of n-heptane/air mixture initiated by a hot spot in 1D planar and spherical systems is numerically investigated considering detailed chemistry. It is found that at low temperature, n-heptane/air mixture undergoes a three-stage ignition process, which is sequentially dominated by low-, intermediate- and high-temperature ignition. At proper temperature gradient, these three ignition stages may all couple with corresponding pressure waves and either generate detonation wave or cause autoignition in front of the propagating reaction front. The complex wave phenomenon of n-heptane/air mixture indicates the significant difference between the ignition modes of large hydrocarbon fuels at low temperature and those of simple fuels or large hydrocarbon fuels at high temperature.

Acknowledgements

This work was supported by National Natural Science Foundation of China (Nos. 51322602 and 51136005) and State Key Laboratory of Engines at Tianjin University (No. K2014-01).

References

- [1] Pan JY, Shu GQ, and Wei HQ. (2014). Interaction of Flame Propagation and Pressure Waves during Knocking Combustion in Spark-Ignition Engines. *Combust. Sci. Technol.* 186: 192-209.
- [2] Kalghatgi GT. (2014). Developments in internal combustion engines and implications for combustion science and future transport fuels. *Proc. Combust. Inst.* 35 In Press. DOI: 10.1016/j.proci.2014.10.002.
- [3] Zaccardi J, Duval L, and Pagot A. (2009). Development of specific tools for analysis and quantification of pre-ignition in a boosted SI engine. *SAE International Journal of Engines*. 2: 1587-1600.
- [4] Wang Z, Liu H, Song T, Qi Y, He X, Shuai S, and Wang J. (2014). Relationship between super-knock and pre-ignition. *Int. J. Engine Res.* DOI: 10.1177/1468087414530388.
- [5] Heywood JB, *Internal Combustion Engines Fundamentals* 1988, New York: McGraw Hill.
- [6] Bradley D. (2012). Autoignitions and detonations in engines and ducts. *Philos. Trans. R. Soc. A*. 370: 689-714.
- [7] Zeldovich YB. (1980). Regime Classification of an Exothermic Reaction with Nonuniform Initial Conditions. *Combust. Flame*. 39: 211-214.
- [8] Clarke JF. (1989). Fast Flames, Waves and Detonation. *Prog. Energy Combust. Sci.* 15: 241-271.
- [9] Bradley D. (1996). 'Hot spots' and gasoline engine knock. *J. Chem. Soc. Faraday Trans.* 92: 2959-2964.
- [10] Weber HJ, Mack A, and Roth P. (1994). Combustion and Pressure Wave Interaction in Enclosed Mixtures Initiated by Temperature Nonuniformities. *Combust. Flame*. 97: 281-295.
- [11] Gu XJ, Emerson DR, and Bradley D. (2003). Modes of reaction front propagation from hot spots. *Combust. Flame*. 133: 63-74.
- [12] Bradley D, Morley C, Gu XJ, and Emerson DR. (2002). Amplified pressure waves during autoignition: relevance to CAI engines. *SAE Technical Paper* 2002-01-2868.

- [13] Kurtz MD and Regele JD. (2014). Acoustic timescale characterisation of a one-dimensional model hot spot. *Combust. Theory Model.* 18: 532-551.
- [14] Dai P, Chen Z, Chen SY, and Ju YG. (2014). Numerical experiments on reaction front propagation in n-heptane/air mixture with temperature gradient. *Proc. Combust. Inst.* 35 In Press. DOI: 10.1016/j.proci.2014.06.102.
- [15] Bradley D and Kalghatgi GT. (2009). Influence of autoignition delay time characteristics of different fuels on pressure waves and knock in reciprocating engines. *Combust. Flame.* 156: 2307-2318.
- [16] Law CK and Zhao P. (2012). NTC-affected ignition in nonpremixed counterflow. *Combust. Flame.* 159: 1044-1054.
- [17] Zhao Z, Chaos M, Kazakov A, and Dryer FL. (2008). Thermal decomposition reaction and a comprehensive kinetic model of dimethyl ether. *Int. J. Chem. Kinet.* 40: 1-18.
- [18] El-Asrag HA and Ju YG. (2014). Direct numerical simulations of NO_x effect on multistage autoignition of DME/air mixture in the negative temperature coefficient regime for stratified HCCI engine conditions. *Combust. Flame.* 161: 256-269.
- [19] Ju YG, Sun WT, Burke MP, Gou XL, and Chen Z. (2011). Multi-timescale modeling of ignition and flame regimes of n-heptane-air mixtures near spark assisted homogeneous charge compression ignition conditions. *Proc. Combust. Inst.* 33: 1245-1251.
- [20] Yoo CS, Lu TF, Chen JH, and Law CK. (2011). Direct numerical simulations of ignition of a lean n-heptane/air mixture with temperature inhomogeneities at constant volume: Parametric study. *Combust. Flame.* 158: 1727-1741.
- [21] Luong MB, Luo ZY, Lu TF, Chung SH, and Yoo CS. (2013). Direct numerical simulations of the ignition of lean primary reference fuel/air mixtures with temperature inhomogeneities. *Combust. Flame.* 160: 2038-2047.
- [22] Chen Z, Burke MP, and Ju YG. (2009). Effects of Lewis number and ignition energy on the determination of laminar flame speed using propagating spherical flames. *Proc. Combust. Inst.* 32: 1253-1260.
- [23] Chen Z. (2010). Effects of radiation and compression on propagating spherical flames of methane/air mixtures near the lean flammability limit. *Combust. Flame.* 157: 2267-2276.
- [24] Chen Z, Burke MP, and Ju YG. (2011). On the critical flame radius and minimum ignition energy for spherical flame initiation. *Proc. Combust. Inst.* 33: 1219-1226.
- [25] Liu SL, Hewson JC, Chen JH, and Pitsch H. (2004). Effects of strain rate on high-pressure nonpremixed n-heptane autoignition in counterflow. *Combust. Flame.* 137: 320-339.