



Experimental and kinetic comparative study on ignition characteristics of 1-pentene and *n*-pentane



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HIGHLIGHTS

- Ignition delay times of 1-butene and *n*-pentane were measured in a shock tube.
- NG model, JetSurF2.0 model and Touchard model were validated.
- NG model was updated to form Aramco-NG model.
- Ignition delay times of 1-pentene and *n*-pentane were compared and the crossover of ignition delay times were explained.

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ABSTRACT

Ignition delay times of 1-pentene and *n*-pentane were measured using a shock tube at pressures from 0.12 MPa to 1.0 MPa, at equivalence ratios from 0.5 to 2.0 with 0.5% and 1.0% fuel concentrations, in the temperature range of 1040–1880 K. Correlations of 1-pentene and *n*-pentane ignition delay times were deduced from the experimental data using a multiple linear regression. A NG model, JetSurF2.0 model and Touchard model were used to simulate the experiments but the performance was not good for all data. The C1–C4 sub-model of the NG model was updated using Aramco Mech 1.3, forming the Aramco-NG model, which conformed closely to the experiments. A crossover of the ignition delay times of 1-pentene and *n*-pentane can be observed in the correlations and calculations as well as in the experimental data. The shorter ignition delay times of 1-pentene in the relative low temperature region can be explained by the abundant H atom producing channels and the higher rate constant of the unimolecular decomposition reaction in this region. In the relative high temperature region, the higher amount of allyl radical formed through the breakage of the C_γ–C_δ bond and lower concentration of oxygen may contribute to the longer ignition delay times for 1-pentene compared with *n*-pentane.

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1. Introduction

Ignition delay time, which can affect the performance and operation of the combustion equipment, is one of the most important parameters in the combustion process. Furthermore, it can be used to validate and establish the chemical kinetic models, which could help to ascertain the detailed combustion process, evaluate the impact on the environment and develop new combustion strategies. Up to now, many studies have been carried out on the auto-ignition of hydrocarbons, but most of them have been focused on the C1–C4 hydrocarbons, especially on the alkenes. While larger hydrocarbons are the important constituents of the real fuels which are widely used in combustion devices, such as internal

combustion engines. Specifically, alkenes are the important component of the real gasoline compositions [1–4] and the proportion of them can be up to 20% [5]. Due to their higher octane number compared with the paraffins, the existence of olefins may contribute to the auto-ignition chemistry. Besides, they also affect the formations of pollutants, especially soot formation in engines [6–8] due to their unsaturation. In recent studies [9,10], four-component gasoline surrogate models including iso-octane, *n*-heptane, toluene and pentene have been formulated. Kukkadapu et al. [11] reported that the four-component models had the closer ignition delay times to the gasoline when compared with three-component models without pentene.

For many years, the studies of alkenes have been limited to the lighter ones such as ethylene [6,12–18], propene [19–23] and butene [24–28]. For pentene, the oxidation of 1-pentene was experimentally studied by Prabhu et al. [29] in a plug flow reactor between 657 K and 714 K. Alatorre et al. [30] conducted

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experiments of the fuel rich 1-pentene–O₂–Ar flame at 50 mbar and simulated their own work. Subsequently, an experimental comparison study of the ignition delay time of 1-pentene and pentane between 600 K and 900 K was carried out by Minetti et al. [31] in a rapid compression machine (RCM) and 1-pentene presented less reactivity in this region. In the following work by Ribaucour et al. [32], these data were used to develop a chemical kinetic model. Later, Touchard et al. [33] investigated the high temperature (from 1130 K to 1620 K) auto-ignition of 1-pentene in a shock tube with equivalence ratios of 0.5 to 2.0 and pressures from 0.73 to 0.95 MPa. A detailed high temperature kinetic model was generated by a mechanism producing software EXGAS. A low temperature kinetic model for the oxidation of 1-pentene and 1-hexene was also proposed by Touchard et al. [34] using the same software EXGAS. Mehl et al. [1] explored the ignition behaviors of the unsaturated hydrocarbons with shock tube and a kinetic model was also developed. Recently, Westbrook et al. [35] studied the oxidation of 2-methyl-2-butene in shock tube and jet-stirred reactor (JSR), and a detailed chemical kinetic model was established based on these experimental data. *n*-pentane, which is the saturated hydrocarbon in the same carbon number with 1-pentene, is also a component of gasoline. Several research has been performed on *n*-pentane using RCMs [31,36,37], shock tubes [37–39], a well-stirred reactor [40] and a flow reactor [29].

Both 1-pentene and *n*-pentane are linear hydrocarbons with 5 carbons and the only difference between them is that 1-pentene has a C=C double bond between the α and β carbon ($C_{\alpha} = C_{\beta} - C_{\gamma} - C_{\delta} - C_{\epsilon}$). Thus, the difference between 1-pentene and *n*-pentane is only produced by the double bond and the comparison between them can help to clarify the property of the double bond. Additionally, the comprehension of the double bond could help to understand the characteristics of unsaturated fatty acid esters, which are the major components of biodiesels. Although some research has been conducted on the ignition characteristics of 1-pentene and *n*-pentane, the data are still limited. Besides, the comparison study of 1-pentene and *n*-pentane is limited to the low temperature region and the mechanism used is not a fully developed one which lacks some reactions such as abstractions of alkyl H-atoms [34]. To further understand the ignition characteristics introduced by the double bond and provide more experimental data to establish the accurate model, the experimental and chemical kinetic modeling studies have been conducted on 1-pentene and *n*-pentane in a shock tube at different equivalence ratios, pressures and temperatures.

2. Experimental section

The experiments were conducted on a shock tube with an effective diameter of 11.5 cm and detailed description of this experimental facility has been reported in the previous literature [41–43]. Thus only a brief introduction of the experimental apparatus and data processing is provided here. The shock tube includes a 4 m long driver part and 5.3 m long driven part, separated by the different thicknesses of polyester terephthalate diaphragms to achieve different reflected pressures. Four fast-response pressure transducer (PCB 113B26) are installed along the last 1.5 m side wall of the driven part with equal spacing and three timers (FLUKE, PM6690) are used to determine the endwall incident shock velocity by linear extrapolation. The endwall pressure and local OH* chemiluminescence are detected by a piezoelectric pressure transducer (PCB113B03) and a photo multiplier (Hamamtsu, CR 131), respectively. In this study, 1-pentene (analytical standard, supplied by Fluka), *n*-pentane (99.5% pure, supplied by Energy Chemical), oxygen (99.99% pure) and argon (99.99% pure) were prepared in a 128 L stainless steel tank with the partial pressures method and at least 12 h was left for homogeneous mixing.

The interval between the shock wave arrival and the extrapolation of the maximum slope line of the OH* signal to the baseline is defined as the measured ignition delay time. A example of ignition delay time definition is shown in [Supplementary Material 1](#). The temperature behind the reflected shock wave was calculated with the reflected shock model by Gaseq [44]. Besides, the uncertainty of temperature in this study is less than 23.7 K and that of the measured ignition delay times is within 15.6%.

3. Results and discussions

3.1. Measurements and correlations

For 1-pentene, ignition delay times were measured at two pressures (0.12 MPa and 1.0 MPa) and three equivalence ratios (0.5, 1.0 and 2.0) behind reflected shock waves in temperature range of 1040–1880 K with a fixed fuel concentration of 0.5%. In addition, experiments were also carried out at the stoichiometric equivalence ratio and 0.1 MPa with fuel concentration of 1.0% for the experimental validation. Prior to current experiments, reproducing experiment was conducted for 1-pentene ignition at 0.1 MPa and good consistency of current data and data from Mehl [1] validate the our facility. For *n*-pentane, experiments were conducted at three equivalence ratios (0.5, 1.0 and 2.0) additionally with the stoichiometric equivalence ratio at 0.12 MPa. The compositions of the test fuel mixtures are listed in [Table 1](#). All the raw data and the validation results are also provided in the [Supplementary Material 1 and 2](#). For all the test fuel mixtures, the ignition delay times exhibit a strong Arrhenius temperature dependence and correlations of the ignition delay time as a function of the equivalence ratio, pressure and temperature are given through the multiple linear regression, with the following form:

$$\tau = A\phi^{\alpha}p^{\beta}\exp(E_a/RT) \quad (1)$$

where τ is the ignition delay time (μ s), ϕ is the equivalence ratio, p is the pressure (MPa), E_a is the global activation energy (kJ/mol), T is the temperature (K) and $R = 8.314 \times 10^{-3} \text{ kJ mol}^{-1} \text{ K}^{-1}$ is the universal gas constant. The parameters (A , α , β , E_a) in the correlations and the fitting factors (R^2) for 1-pentene and *n*-pentane are given in [Table 2](#).

[Fig. 1](#) shows the experimental data and fitted values calculated by Eq. (1). It can be seen that the correlations agree well with the experimental data. As expected, for both 1-pentene and *n*-pentane, ignition delay times increase with the equivalence ratio and decrease with pressure, indicating plus and minus sign of their index, respectively. Furthermore, compared with *n*-pentane, 1-pentene exhibits longer ignition delay times at higher temperatures and shorter ignition delay times at relative low temperatures. The crossover of the ignition delay time results in the lower activation energy of 1-pentene (as shown in [Table 2](#)).

3.2. Chemical kinetic model validation

Simulations were carried out with the Chemkin II package [45], using the Senkin code [46] with a zero-dimensional and constant

Table 1
Compositions and pressure conditions of test mixtures in this study.

Fuel	Fuel (%)	O ₂ (%)	Ar (%)	ϕ	p (MPa)
1-pentene	1	7.5	92	1.0	0.1
	0.5	7.5	92.0	0.5	1.0,0.12
	0.5	3.75	95.75	1.0	1.0,0.12
	0.5	1.875	97.625	2.0	1.0,0.12
<i>n</i> -pentane	0.5	8	91.5	0.5	1.0
	0.5	4	95.5	1.0	1.0,0.12
	0.5	2	97.5	2.0	1.0

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