

## Full Length Article

# Experimental and kinetic modeling study on 2,4,4-trimethyl-1-pentene ignition behind reflected shock waves



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## HIGHLIGHTS

- The ignition delay times for 2,4,4-trimethyl-1-pentene were measured.
- The only chemical kinetic model (Metcalfe model) was validated and optimized.
- The sensitivity analysis and reaction pathway analysis were performed.

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## ABSTRACT

Experiments of ignition delay times on 2,4,4-trimethyl-1-pentene were performed behind reflected shock waves at pressure ranging from 2 atm to 10 atm, at equivalence ratios from 0.5 to 2.0, and with fuel concentrations of 0.5%, 0.75% and 1%. All ignition delay times follow the Arrhenius rule, and discussions on the effect of pressure, temperature, equivalence ratio and fuel concentration on ignition delay times were made. Metcalfe model overpredicts the ignition reactivity of 2,4,4-trimethyl-1-pentene, and this model was modified to achieve better agreement for measured ignition delay times. Sensitivity analysis and reaction pathway analysis were conducted to gain a deep insight into 2,4,4-trimethyl-1-pentene ignition chemistry. The ignition delay time is sensitive to the small-radical reactions. In addition, H abstraction reactions and unimolecular decomposition reactions dominate the ignition process.

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## 1. Introduction

Gasoline consists of hundreds of hydrocarbons [1–4], with major components of paraffins, naphthenes (cycloparaffins), olefins and aromatics, etc. Due to the complexity of real gasoline components, gasoline surrogates are used to the simulation of the internal combustion engines. Thus the chemical kinetic mechanism of gasoline surrogates plays a significant role on the combustion and emission simulation of practical internal combustion engines. Simulations with chemical kinetic mechanism can optimize engine combustion strategies, reduce pollutant emissions and improve engine efficiency. Therefore, the development of chemical kinetic mechanism of gasoline surrogate is necessary to the design and optimization of internal combustion engines.

Gasoline surrogates are composed of several representative components to predict characteristics of gasoline, such as combustion behavior [5–7], evaporation and thermodynamic properties.

The simplest surrogate fuel consists of single component, such as iso-octane. In addition, binary mixtures consisting of iso-octane and *n*-heptane called primary reference fuels (PRF) was proposed and extensively studied [7–9]. Iso-octane and *n*-heptane were selected to stand for saturated branched alkanes and saturated linear alkanes, respectively. In a recent review [10], toluene was chosen as a third component to add to PRF to match the gasoline properties. This mixture is called toluene reference fuel (TRF) and numerous kinetic models for it was developed [11,12]. In addition to ternary surrogates, quaternary surrogates consisting of TRF and alkenes have been reported [13–15]. For the alkene component, diisobutylene (consisting of two conjugate olefins of iso-octane: 2,4,4-trimethyl-1-(and -2-) pentene) is chosen as a representative of highly branched alkenes.

Some researches on combustion and emission characteristics of diisobutylene and gasoline surrogates containing diisobutylene have been performed in practical internal combustion engine. Kaiser et al. [16] studied the emissions of neat diisobutylene and diisobutylene/gasoline blends in a spark ignition engine. The results showed that emissions could be related to the concentration of diisobutylene in the fuel blends. Ninomiya and Golovoy

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[17] explored the effects of air-fuel ratio on composition of hydrocarbon exhaust from pure isooctane, diisobutylene, toluene and toluene-*n*-heptane mixture in a single-cylinder engine. The results showed that iso-octane and diisobutylene combustion produces large concentrations of olefins in exhaust. Shibata et al. [18] investigated combustion behaviors of eighteen kinds of two hydrocarbon blended fuels, which were composed of *n*-heptane and another hydrocarbon, such as iso-octane, diisobutylene, 4-methyl-1-pentene, toluene or cyclopentane in HCCI engine. They observed that *n*-heptane/diisobutylene blends shows less noticeable two-stage ignition behavior than *n*-heptane/toluene blends. Rankovic et al. [19] investigated the effect of diisobutylene addition into gasoline surrogates on research octane number (RON) in a CFR engine. Their study showed a non-linear behavior of RON with respect to the volume of diisobutylene addition.

For the fundamental combustion research on diisobutylene, ignition delay times of quaternary gasoline surrogates including 10% diisobutylene were measured in high-pressure shock tube under various conditions by Fikri et al. [20] These data were utilized to develop a detailed kinetic model for gasoline surrogate fuels by Andrae [21]. Later, Canino et al. [22] explored the ignition behaviors on quaternary gasoline surrogates with 13% diisobutylene under stoichiometric conditions by shock tube, proposing a chemical kinetic model. Besides, Mittal and Sung [23] measured ignition delay times of binary blends of three surrogate components for gasoline, including iso-octane, 2,4,4-trimethyl-1-pentene and toluene in a rapid compression machine at 850–1050 K. The results showed that 2,4,4-trimethyl-1-pentene addition to toluene makes longer ignition delay than iso-octane addition. A semidetached chemical kinetic model of a quaternary gasoline surrogate consisting of *n*-heptane, iso-octane, toluene and diisobutylene was proposed by Wang et al. [24]. And recently a kinetic model combined the quaternary gasoline surrogate with ethanol was also established by Zhong et al. [25]. Samimi et al. [26] proposed a chemical kinetic model of seven-component gasoline surrogates including diisobutylene. This model gives good predictions on ignition delay time, laminar flame speed and distillation curve data.

Until now, there are very limited fundamental combustion research on neat diisobutylene. Metcalfe et al. [27] measured ignition delay time of diisobutylene isomers (both 2,4,4-trimethyl-1-pentene and 2,4,4-trimethyl-2-pentene) with shock tube at 1–4 atm and at equivalence ratios of 0.25, 0.5, and 1.0. A chemical kinetic model were also established and this model under-predicted the experimental data at higher temperature conditions.

Therefore, although diisobutylene is a potential fuel for the gasoline surrogates, the kinetic study on neat diisobutylene has not been adequately investigated. The ignition delay time of diisobutylene are still limited to lower pressure region and fuel lean mixtures. In addition, the only kinetic model need to be further optimized.

The objectives of this study are to measure ignition delay times of diisobutylene at wide initial conditions and optimize the Metcalfe's kinetic model. Reaction pathway and sensitive analysis were conducted to gain better understanding into 2,4,4-trimethyl-1-pentene ignition processes.

## 2. Experimental section

### 2.1. Experimental method

All measurements presented in this study were obtained in a shock tube described in detail in Refs. [28–31]. Briefly, this shock tube with 11.5 cm internal diameter consists of a 5.3 m long driven section and a 4.0 m long driver section. These two parts are sepa-

rated by a double PET (Polyethylene terephthalate) diaphragms. Before each test, the shock tube was evacuated below 1.0 Pa and the leak rate was less than 1.0 Pa/min which can be negligible. Reactant mixtures (argon, oxygen, 2,4,4-trimethyl-1-pentene of 99.995%, 99.995%, 99% purities, respectively) were prepared in a 128L stainless steel tank according to the partial pressure method and should be settled more than 4 h for homogeneous mixing. Four pressure transducers (PCB, B26) are located along the last 1.5 m side-wall to trigger time counters. The time instant of the shock wave arrival at each pressure transducer location is sent to three time counter (Fluke PM6690), so that the shock wave velocity profile along the shock tube direction is determined. A pressure transducer (PCB 113B03) is also mounted at the end wall to measure the end wall pressure. Temperature behind the reflected shock wave is calculated with Gaseq [32]. In addition, a photomultiplier (Hamamatsu CR 131) is located at the endwall to measure CH\* emission signal selected by a  $306 \pm 10$  nm narrow filter. All data are recorded in a digital recorder (Yokogawa, ScopeCorder DL750).

Fig. 1 shows the relative pressure and CH\* emission signal. The definition of ignition delay time is the time duration between the arrival of the shock wave at the endwall and the extrapolation of the sharpest rise in the CH\* emission signal to the zero baseline. The compositions of mixtures are summarized in Table 1. Experiments of 2,4,4-trimethyl-1-pentene were conducted at equivalence ratios of 0.5, 1.0, 2.0, pressure of 2–10 atm.

### 2.2. Uncertainty analysis

The uncertainty of ignition delay time is conducted from the uncertainties of pressure, equivalence of ratio, fuel mole fraction, and temperature. In general, the uncertainties of fuel concentration and equivalence ratio can be limited to 1% and could be neglected. Therefore, the uncertainty of ignition delay times mainly comes from measurements of temperature and pressure. For temperature uncertainty, it is caused by the uncertainty of incident shock tube wave velocity, which is determined by time intervals recorded by timer counters and the distances between pressure transducers. 1000 ns of uncertainty of time interval is estimated, which is determined by the resolution time of pressure transducer. In addition, the uncertainty of distances is estimated as follows. It mainly comes from the resolution of pressure transducer, the diameter of the sensing area of the transducer and the shock front thickness. Here, the value of the distance uncertainty origin from the resolution of pressure transducer is estimated as the product of the resolution time and the shock velocity, i.e.  $1000 \text{ ns} \times V_s$ .  $V_s$  is the shock tube wave velocity. Because the trigger position of shock

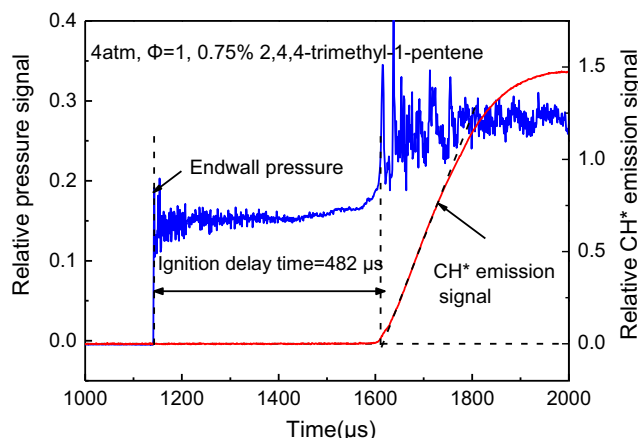


Fig. 1. Definition of ignition delay time.

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