



Full Length Article

Autoignition of ternary blends for gasoline surrogate at wide temperature ranges and at elevated pressure: Shock tube measurements and detailed kinetic modeling



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HIGHLIGHTS

- Three ternary gasoline surrogates with the same RON95 were constructed.
- Ignition delay of four toluene reference fuels was measured in shock tube.
- A detailed chemical kinetic model for the ternary gasoline surrogates was established.
- The ignition properties and reaction pathways of TRFs were analyzed.
- A comparison of ignition characteristics of toluene reference fuels with same RON was made.

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ABSTRACT

Considering the diverse compositions of commercial gasoline, the ignition delay time of toluene reference fuels (TRF) composed of isooctane, n-heptane and toluene was studied in a shock tube under the conditions of medium to high temperature ranges, different pressures (10–20 bar), and various equivalence ratios (0.5, 1.0, 1.5 and 2) by reflected waves. To analyze the impacts of the component proportion on the gasoline surrogate combustion process, three different ternary blends, TRF2 (42.8% isooctane/13.7% n-heptane/43.5% toluene), TRF3 (65% isooctane/10% n-heptane/25% toluene) and TRF4 (87.2% isooctane/6.3% n-heptane/6.5% toluene), with the same Research Octane Number of 95 (RON = 95) were constructed; TRF1 was the same as Surrogate A in Gauthier et al. (2004). The experimental results showed that there was an obvious negative correlation between the ignition delay time of the toluene reference fuels and the pressure, temperature and equivalence ratio; notably, the measured data showed a minimal discrepancy of TRF2, TRF3, and TRF4 at pressures of 10 and 20 bar in a stoichiometric ratio. Based on Curran's (2002) detailed kinetic model for PRF (primary reference fuel) and Yuan's (2015) toluene pyrolysis and oxidation model, which updated and integrated the thermodynamic parameter and reaction rate for some key reactions, a detailed chemical mechanism consisting of 1251 species and 5705 reactions was established to illustrate the surrogate combustion properties. The model captured the autoignition behavior of all four ternary gasoline surrogates well in the shock tube experiments, especially at high pressure and under rich fuel conditions. Furthermore, the sensitivities and a reaction pathway analysis were also calculated for different blending ratios using CHEMKIN-PRO software, which exhibited and analyzed partial ignition features with respect to the chemical reactions based on the model proposed in this work.

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1. Introduction

For the past several decades, increasing numbers of new-type combustion modes have been at the center of worldwide innovation and research focus, with increasingly urgent requests for

high-efficient and zero-emission internal combustion engine (ICE), more combustion modes [1–6] with highly efficient, ultra-low NO_x and soot emissions also are in the charge of chemical kinetics are promoted. To this end, it's imperative to exactly determine the detailed chemical mechanism of fuels in ICE operation conditions.

However, study of the chemical kinetics of multicomponent fuel is still immature and limited due to the computing resources. As a

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result, the construction of a detailed mechanism model for petrochemical fuel, which commonly contains thousands of hydrocarbons and varies with seasons and places of origin, is not feasible. Therefore, establishing a gasoline surrogate mechanism model involving limited components is turning into research emphasis, in accordance with the carbon distribution and fundamental family of the chemical constituents of the modeling goals. In addition, not only physical properties (such as the density, the viscosity and the evaporation characteristics) but also chemical properties (such as the octane number/cetane number, the C/H, the flame speed and the adiabatic flame temperature) should be matched by the surrogate. Hence, a series of foundation experimental facilities, such as ST (shock tubes), RCM (rapid compression machines), JSR (jet-stirred reactors), FL (flow reactors), combustion bombs and single-cylinder engines, have been adopted to investigate the combustion features of gasoline surrogates and to validate relevant chemical kinetic models.

Gasoline is a complex mixture comprising branched paraffin, olefins, cycloparaffins and aromatics [7,8], which contains 4–13 carbons. Due to its high octane number, isooctane was first selected to represent real unleaded gasoline as a surrogate. Curran et al. [9] at the LLNL (Lawrence Livermore National Laboratory) constituted a detailed chemical kinetic model (858 species and 3606 reactions) for isooctane oxidation, followed by a series of skeleton and reduced mechanism afterward [10–12]. Even though isooctane can represent gasoline properties to some extent, it cannot reproduce the combustion process and specific emission characteristics of commercial gasoline. Increasing attention has been focused on PRF (primary reference fuel), a binary gasoline surrogate that can achieve a variety of gasoline octane number flexibly by mixing isooctane and n-heptane in a certain ratio. Curran et al. [13] utilized an ST and a high pressure FL to measure the autoignition and combustion intermediate concentrations at 690–1220 K, 40 atm and 550–880 K (12.5 atm individually) and founded and confirmed the detailed kinetics model for PRF (1034 species and 4238 reactions), and Chaos et al. [14] reduced it with only the high temperature (>950 K) and low pressure condition (<15 atm) therein, while Andrae et al. [15] added 132 co-oxidation reactions of two ingredients to it, updating the model to a new form that could satisfy the PRF80 (80% isooctane) ignition delay in HCCI combustion conditions. Moreover, Tanaka et al. [16], Ra and Reitz [17], Tsurushima [18] and Neshat and Saray [19] also developed their own reduced kinetic model of PRF.

The long-term study of PRFs with the same RON and MON (Motor Octane Number) largely promoted the development of the gasoline surrogate chemical kinetic model, in spite that it could not match commercial gasoline sensitivity (S , $S = \text{RON} - \text{MON}$), whose numerical value causes deviation in the autoignition behavior. Because there is a relatively high proportion of aromatics in commercial gasoline and their contribution to soot precursors, an increasing number of researchers have focused on the experimental study of toluene [20,21], especially the autoignition behavior of it [22–25], meanwhile, they also devoted themselves to developing the toluene chemical mechanism [26–28], in light of the updated decomposition channels and reaction rates [29–32]. However, it is obvious to see that most of the toluene mechanism models only center on the oxidation process of toluene. Recently, Yuan et al. [33,34] used SVUV-PIMS to research the pyrolysis of toluene at pressures from 5 to 76 Torr and temperatures from 1100 to 1730 K, and measured the concentration profiles of the pyrolysis species and intermediates, while the oxidation of toluene in a JSR was studied by GC combined with flame ionization detector (FID), thermal conductivity detector (TCD) and MS; he also proposed and corroborated a detailed kinetic model of toluene pyrolysis and oxidation (272 species and 1698 reactions), including the chemistry of aromatics growth

by miscellaneous methods, which is the most detailed and accurate chemical model thus far.

On the basis of the development of the toluene chemical kinetic model, TRF (toluene reference fuel) was kept drawing attention by researchers. Gauthier et al. [8] found that the ignition delay of a TRF named Surrogate A was consistent with the corresponding commercial gasoline RD387 ($(\text{RON} + \text{MON})/2 = 87$) and confirmed that TRF is an efficient gasoline surrogate, and Andrae et al. [35–37] built and reduced a detailed kinetic model of TRF by combining PRF, toluene, benzene [38] sub-mechanism and cross-reactions together, moreover, Saikai et al. [39], Niemeuer and Sung [40] and Wang et al. [41] conducted a series of research on the reduced chemical mechanism of TRF. Furthermore, more and more scholars like Bruce et al. [42–44] are committed to applying surrogates contained TRF in experiments and simulations of engines under various operation modes with the improvements of basic experiments and the chemical kinetic model for gasoline surrogates.

Therefore, the tendency of gasoline surrogates is to pursue high reproduction in more respects of gasoline characteristic with limited components when the size of its matching chemical mechanism becomes progressively smaller, which makes the ternary blends for gasoline surrogates mixed with isooctane, n-heptane and toluene increasingly vital. Considering the diverse components in commercial gasoline that change with the seasons and origins, the present study established three ternary blends for gasoline surrogates, named TRF2/TRF3/TRF4, with the same compositions and RON (RON = 95) by different blending ratios, aimed at investigating the effects of proportion on the autoignition behavior of the surrogates in an ST. In addition, a detailed chemical kinetic model of TRF, based on Curran's [13] and Yuan's [33,34] chemical kinetic model of PRF and toluene, respectively, was proposed and validated in this study, and the model was used to study the relationship between the combustion characteristics of TRF and the pressure, temperature and equivalence ratio.

2. Experimental approach

2.1. Shock tube apparatus and the definition of the ignition delay

The specific description and reliability analysis of all measurements carried out in an ST are provided in Refs. [45,46], and a brief introduction is given here. The entire ignition delay time experiments in this study were performed in a 90-mm inner diameter, unheated, high purity, helium-driven shock tube facility. Six piezo-electric pressure transducers (PCB113B26) were positioned axially along the driven section, which was used to record the arrival of the incident and reflected wave, whereas the OH^* emission was detected by a photomultiplier (Hamamatsu, R928). The purities of all gases used in this study were 99.999%, toluene and isooctane were 99.5%, and n-heptane was 99.9%. To ensure sufficient blending, all fuels were mixed with synthetic air ($\text{N}_2:\text{O}_2 = 3.76:1$) in a stainless-steel tank for at least 12 h at room temperature before the experiments at every operation condition.

The definition of the ignition delay is different for kinds of experimental facilities even for various STs used by each research group. Commonly, the combustion pressure undergoes a sudden rise when the fuels are ignited, yielding a tremendous amount of OH^* and CH^* in the meantime. Thus the pressure history, OH^* and CH^* are often regarded as the symbols of ignition, which generally agree to within $\pm 5\%$ [25]. However, every research group still has its precise definition of the ignition delay: Pitz et al. [26] and Bounaceur et al. [28] defined the ignition delay as the time interval between the pressure rise measured by the last pressure transducer when the reflected shock wave arrived and

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