



Homogeneous charge compression ignition of binary fuel blends

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Abstract

The present experimental investigation aims to understand the homogeneous combustion chemistry associated with binary blends of three surrogate components for practical fuels, including toluene, isooctane, and diisobutylene-1 (DIB-1). Specifically, high-pressure autoignition characteristics of the three neat fuel components as well as the fuel blends of toluene + isooctane and toluene + DIB-1 are studied herein. Experiments are conducted in a rapid compression machine at compressed pressures varying from 15 to 45 bar and under low to intermediate temperatures. To obtain insights into interactions among fuels, the relative proportion of the two neat fuels in the reactive mixtures is systematically varied, while the total fuel mole fraction and equivalence ratio are kept constant. Experimental results demonstrate that ignition delays for neat toluene are more than an order of magnitude longer than those for neat isooctane. Whereas DIB-1 has ignition delays shorter than those for isooctane at higher temperatures, at temperatures lower than 820 K DIB-1 shows a longer ignition delay. Although the ignition delays of binary blends lie in between the two extremes of neat components, the variation of ignition delay with the relative fuel proportion is seen to be highly nonlinear. Especially, a small addition of isooctane or DIB-1 to toluene can result in greatly enhanced reactivity. In addition, the effect of DIB-1 addition to toluene is more significant than the effect of isooctane addition. Furthermore, in the compressed temperature range from 820 to 880 K, ignition delay of the toluene + isooctane blend shows greater sensitivity to temperature than that of isooctane.

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1. Introduction

Practical liquid fuels contain hundreds of hydrocarbons, which complicates the development of a kinetic mechanism of reasonable size for large-scale computation. The use of surrogate fuels is a viable ap-

proach to make the development of chemical kinetic mechanisms for practical fuels tractable. A surrogate fuel model that consists of a small number (usually less than 10) of fuel components can be developed to represent the real fuel and predict the desired characteristics of the actual fuel. One approach to developing a fuel surrogate is to use a single component from each hydrocarbon class in the practical fuel so that the unique molecular structure of each class is included. Therefore, the reaction mechanisms of individual fuel

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components typically provide the basis for the development of surrogate kinetic models, and the accuracy of a surrogate model is directly dependent on the validation of the neat component models over a broad range of experimental conditions.

The present experimental investigation focuses on three fuel components, isooctane (2,2,4-trimethylpentane, C₈H₁₈), toluene (methylbenzene, C₇H₈), and diisobutylene-1 (2,4,4-trimethyl-1-pentene, C₈H₁₆). In particular, isooctane and toluene are anticipated as the primary components respectively representing alkanes and aromatics in gasoline surrogates, and are also recognized as components for jet fuel surrogates [1]. In addition, diisobutylene-1 (DIB-1) is identified as a potential candidate for representing alkenes in gasoline surrogates. Recognizing that these classes of hydrocarbons have vast differences in the overall reactivity and autoignition chemistry, and that their behaviors in various blends are not properly understood, we aim to conduct a systematic investigation for neat fuels and their binary blends to characterize the nature of interactions amongst them, with special emphasis on autoignition kinetics at low to intermediate temperatures and high pressures.

It is noted that all three fuel components investigated in the present study have high octane numbers and are relatively resistant to autoignition. At low temperatures, isooctane shows a region of negative temperature coefficient and dominance of peroxidation reactions [2], resulting in faster ignition than for toluene. On the other hand, toluene is well known as being resistant to low-temperature oxidation due to the stability of the benzyl radical. Unlike most alkyl radicals and aromatics with side chains, the benzyl radical has no easy reaction with O₂ to give a conjugate alkene and the HO₂ radical [3]. Due to the enhanced stability of benzyl as a result of delocalization of electrons, H abstraction is also uncompetitive. As a consequence, radical–radical recombination leading to bibenzyl becomes important. In the rapid compression machine (RCM) experiments of Roubaud et al. [4], a stoichiometric mixture of toluene did not autoignite below 916 K at 17 bar. However, oxidation of toluene may take place at lower temperatures when it is present in a blended fuel mixture due to the development of a radical pool formed by the other easily oxidized fuel components in the mixture. DIB-1 has a molecular structure similar to that of isooctane, and therefore its kinetics provides insight into the effect of including a double bond in the carbon skeletal structure of isooctane. Investigations [5] have shown that the inclusion of a double bond and its position can drastically alter the fuel combustion characteristics.

During the combustion of blended fuels, it is also unclear how the interaction of different components can affect the system response. Klotz et

al. [6] observed that independently developed models of toluene and butane, when merged together, could predict the kinetics of blended fuels. While this aspect can greatly simplify the development of reaction mechanism of blended fuels, it is not necessarily a general conclusion. In particular, there can be a possibility of chemical interactions between different fuel components and their radicals, and exclusion of such interactions can place undue restrictions on the reaction pathways. Andrae et al. [7] investigated the autoignition of primary reference fuels (PRFs) and toluene/*n*-heptane blends. In their model validation, interaction reactions between the individual fuel components were found to be important in predicting homogeneous charge compression ignition (HCCI) experiments [7].

Due to chemical interactions in blended fuels, differences in sensitivity of fuels are also recognized. For example, Andrae et al. [7] attributed the difference in sensitivity of a PRF and a toluene/*n*-heptane blend with the same octane number to the effect of interaction reactions. Tanaka et al. [8] found better agreement between model predictions and experimental data by including a coupling reaction between *n*-heptane and isooctane. Therefore, systematic development of surrogate mechanisms and understanding of chemical kinetic processes leading to autoignition requires studies of kinetic interactions in blended fuels.

Although blends of the primary reference fuels, *n*-heptane and isooctane, have been studied extensively, investigations on blends of toluene with isooctane and DIB-1 are meager. Recently, Vanhove et al. [9] conducted experiments focusing on selective binary blends, including toluene + isooctane, in a rapid compression machine at temperatures below 900 K and pressures less than 16 bar. For toluene + isooctane blends, in particular, a large change in the temperature dependences of both the first stage delays and the total ignition delays was noted with addition of toluene to isooctane [9].

This work focuses on the autoignition of toluene + isooctane and toluene + DIB-1 blends at low to intermediate temperatures and elevated pressures, because autoignition chemistry under such conditions has not been well established. Experiments are conducted for various homogeneous mixtures in a rapid compression machine. The specific objective is to obtain extensive experimental data for autoignition of neat fuel components and binary blends under conditions relevant to engine combustion, thereby providing validation targets for model development and developing an understanding of kinetic interactions in the fuel blends. In the following, we shall sequentially present the experimental specifications and discuss our experimental results.

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