Fuel 128 (2014) 458–466

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

A chemical mechanism for ignition and oxidation of multi-component gasoline surrogate fuels

Bei-Jing Zhong *, Dong Zheng

Department of Engineering Mechanics, Tsinghua University, Beijing 100084, PR China

HIGHLIGHTS

- A chemical kinetic mechanism of gasoline surrogate fuels.
- Reduced sub-mechanism of toluene and diisobutylene.
- Predicted ignition delay times and laminar flame speeds.
- Describe the auto-ignition and combustion characteristics of real gasoline.

ARTICLE INFO

Article history:
Received 3 December 2013
Received in revised form 19 March 2014
Accepted 20 March 2014
Available online 2 April 2014

Keywords:
Gasoline surrogate fuels
Chemical mechanism
Ignition
Diisobutylene
Toluene

ABSTRACT

A chemical kinetic mechanism consisting of 89 species and 355 elementary reactions is developed for the prediction of ignition and oxidation behaviors of gasoline surrogate fuels composed of five components, namely, *iso*-octane, *n*-heptane, ethanol, toluene, and diisobutylene. Model validation results show that the predicted ignition delay times and laminar flame speeds of the mechanism are consistent with the experimental results, not only for pure mono-component fuels but also for mixed multi-component gasoline surrogate fuels and real gasoline. The mechanism developed here can correctly describe the auto-ignition and combustion characteristics of real gasoline.

1. Introduction

Gasoline auto-ignition characteristics have a significant effect on the combustion processes of an internal combustion (IC) engine. On the one hand, auto-ignition is a direct factor of knocking in a spark ignition (SI) engine. On the other hand, it is also one of the most essential characteristics of a homogeneous charge compression ignition (HCCI) engine. Combustion of fuel/air mixtures that release heat is a premise in auto-ignition. Auto-ignition is a kinetically controlled process. Therefore, the chemical kinetic mechanism of gasoline must be analyzed.

Gasoline is a multi-component fuel that contains hundreds of hydrocarbons. The composition of gasoline varies with the fuel source and the refinery process it undergoes. Hence, a chemical kinetic mechanism of gasoline cannot be directly developed. Gasoline generally contains linear paraffins, branched paraffins, cyclic paraffins, aromatics, olefins, and oxygenic components [1] and has corresponding representative components of *n*-heptane, *iso*-octane, cyclopentane, toluene, diisobutylene (DIB), and ethanol. A representative component or a blend of several representative components can be regarded as a gasoline surrogate fuel. Surrogate fuels must well describe or reproduce the physical (e.g., density, viscosity, evaporation, etc.) and chemical (e.g., ignition delay time, laminar flame speed, pollutant emission, etc.) properties of gasoline.

Iso-octane is the most common and simplest surrogate of gasoline. Several studies have presented kinetic models of *iso*-octane [2–4]. Among these models, the mechanism proposed by Curran et al. [3] is the most detailed and can well describe the ignition processes. However, models of *iso*-octane are still unable to reproduce the auto-ignition of gasoline because of the high octane number of *iso*-octane. Hence, two-component blends of *iso*-octane and *n*-heptane, also called primary reference fuels (PRFs), are widely accepted and used to represent a gasoline surrogate with different octane numbers. Several kinetic mechanisms of PRFs have been reported in the literature [5–9], among which the reduced PRF mechanism of Ra and Reitz [7] not only presents a smaller scale but also

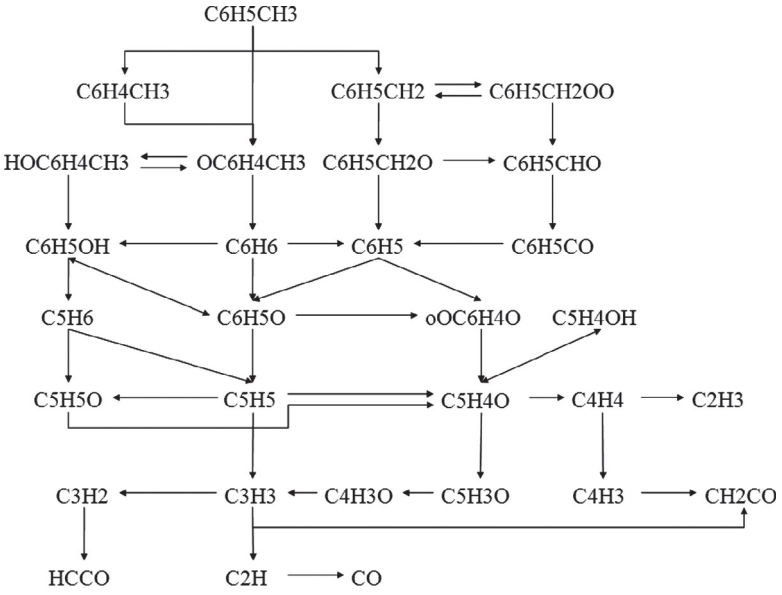
* Corresponding author. Tel./fax: +86 10 62772928.
E-mail address: zhongbj@tsinghua.edu.cn (B.-J. Zhong).

http://dx.doi.org/10.1016/j.fuel.2014.03.044
0016-2361/

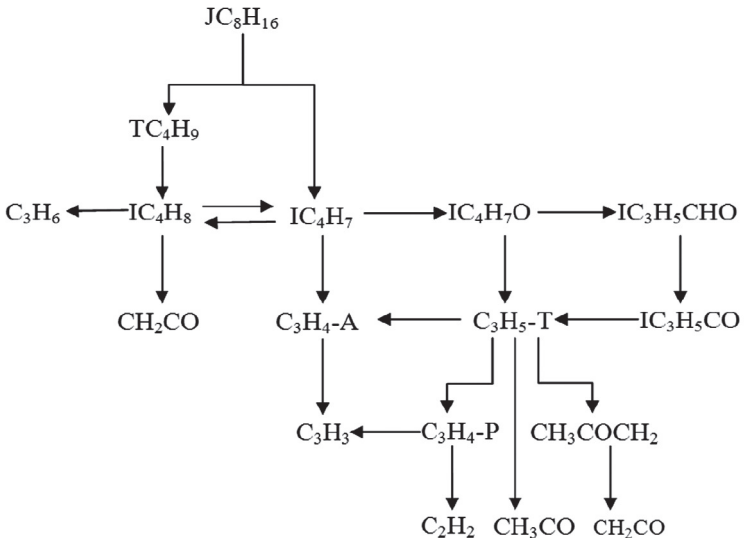
Table 1
The composition (by liquid vol.%) of several gasoline surrogate fuels.

Fuel	*Iso*-octane	*N*-heptane	Toluene	Ethanol	Diisobutylene	RON	Reference
Surrogate A	63	17	20			88	[18]
Surrogate B	69	17	14			87	[18]
Surrogate C	62	18		20		95	[19]
Surrogate D	25	20	45		10	94.6	[19]
Surrogate E	37.8	10.2	12	40		98.8	[20]
Surrogate F	30	22	25	10	13	95.1	[21]

accurately predicts the ignition delay time, cylinder pressure, and heat-release rate of PRF. However, PRF is only suitable for SI engines, not HCCI engines. Therefore, gasoline surrogates should contain more representative components for extensive application. Pitz et al. [10] suggested a three-component fuel consisting of *iso*-octane, *n*-heptane, and toluene, also called toluene reference fuel (TRF), as a gasoline surrogate, and several studies have presented different TRF mechanisms [11–15]. Ethanol and DIB should be introduced to gasoline surrogate fuels because ethanol is regarded as a valuable fuel additive and DIB can represent the olefin components of gasoline. A detailed mechanism with 1,121 species and 4,961 elementary reactions [16] and its reduced mechanism, including 142 species and 672 elementary reactions [17], for a five-component gasoline surrogate fuel composed of



(a) toluene



(b) DIB

Fig. 1. Major reaction branches of fuels oxidation. (a) Toluene; (b) DIB.