



# High-temperature oxidation kinetics of *iso*-octane/*n*-butanol blends-air mixture



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## ABSTRACT

A chemical kinetic mechanism of *n*-butanol/*iso*-octane blends (Model BI) was established on the basis of a *n*-butanol reaction submechanism and part of a high-temperature oxidation mechanism of *iso*-octane. Model BI was validated against laminar flame speeds, ignition delay times and JSR data, and proved to be applicable and reliable. It also found that the laminar flame speed of blends increased linearly and monotonically with the increasing ratio of *n*-butanol. Then detailed kinetic pathway analysis of *n*-butanol/*iso*-octane blends were performed based on Model BI to find out the reason for the accelerating effect of added *n*-butanol. The most influential elementary reactions were determined for the blend, and the laminar flame speed is largely negative related to the concentration of  $iC_4H_8$ ,  $C_3H_6$  and  $CH_3$ , while  $C_2H_4$  and  $C_2H_3$  contribute to the promotion of laminar flame speeds. Flame structures of *n*-butanol blending with *iso*-octane were also computed and correspond to the kinetic pathway analysis.

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## 1. Introduction

Gasoline has played a significant and an irreplaceable role in the current society. However, as fossil fuels are not renewable, searching for alternative fuel is extremely urgent, and bio-alcohols has received great attention in the past decades. Except for ethanol, the most common and dominant addition of gasoline, *n*-butanol is also considered as a promising alternative fuel [1].

Industrialized *n*-butanol production has been proved completely feasible via A.B.E fermentation process, which is the same route of ethanol production. With the development of butanol fermentative process, a higher butanol production rate of A.B.E has become possible [2–4], indicating that *n*-butanol and ethanol share similar renewability. However, as an addition of gasoline, *n*-butanol takes some advantages over ethanol: lower water absorption, better blending ability and less corrosivity to engine system. Furthermore, the thermal physical properties of *n*-butanol are comparable to gasoline, thus it can be used in engines without major modification on the engine structures [5]. Wu et al. [6] reported that the use of single *n*-butanol could achieve

substantial fossil energy savings (39–56%) and induce a reduction in greenhouse gas emissions (32–48%) on a life-cycle basis. Considering the production cost of *n*-butanol is still high, blending *n*-butanol with gasoline is a more realistic option for IC engines. Numerous research on in-cylinder performance of *n*-butanol/gasoline and *n*-butanol/diesel has been conducted on both spark-ignition and compression-ignition engines [7–20].

Dernotte [7] observed that an optimum concentration of 40% butanol in gasoline enables to run the engine at leaner mixture than gasoline. Szwaja et al. [8] conducted research on blends of *n*-butanol/*iso*-octane at different blending ratios, using a single cylinder SI engine with variable compression ratio. Experiments by Rakopoulos et al. [9] and Siwale et al. [17] on a turbocharged diesel engine showed that addition of *n*-butanol could lead to serious smoke, CO reduction but NO increase. However, Valentino et al. [10] observed improvements in both NO<sub>x</sub> and smoke emissions. Broustail et al. [11] carried out experiments of butanol/*iso*octane blends on a single-cylinder port-fuel injection SI engine and found that addition of *n*-butanol results in a strong decrease in HC and NO<sub>x</sub> emissions. Venugopal et al. [13] studied *n*-butanol and gasoline in a dual injection SI engine, and pointed out that injecting *n*-butanol just before the start of injection of gasoline was beneficial for reducing HC and CO emissions. He et al. [18] investigated the low-temperature combustion characteristics of *n*-butanol/*iso*-octane blends and announced that *n*-butanol autoignites more easily than *iso*-octane at low temperature. Yu et al. [19] studied the

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spray–wall impingement characteristics of n-butanol/diesel blends under various environmental condition with different injection strategies. Feng et al. [20] presented a theoretical analysis on the efficiency of blends. It can be figured out that with proper blending ratio and minor adjustment of engine system, addition of n-butanol can result in improvement in thermal efficiency and/or reduction in CO, HC, NOx and soot emissions.

In order to gain a deeper insight into the in-cylinder combustion process of gasoline/n-butanol blends, it's necessary to carry out research on gasoline/n-butanol fundamental combustion characteristics. As the real gasoline composition is too complex and difficult to reproduce, primary reference fuels (PRF) are commonly chosen as the surrogate for the octane ratings of gasoline fuels [21,22]. The vast majority of PRF, especial for high research octane numbers, is iso-octane. For example, PRF90 mixtures indicate that 90% of the mixture is iso-octane. Here, iso-octane is chosen as the surrogate of the real gasoline in the fundamental combustion research. The researches on iso-octane/n-butanol blends using spherically expanding flame are so far very limited and mainly focus on its laminar flame speed measurements [23–26]. For example, Broustail et al. measured the laminar flame speed of butanol/iso-octane blends, and Fu et al. gave the correlation of laminar flame speed of butanol/iso-octane blends on diluent and blend ratio effects.

These measurements revealed that iso-octane/n-butanol blends burn faster than pure iso-octane. To gain an in-depth understanding of this phenomenon, conducting detailed chemical kinetics analysis is indispensable. In the past several years, researches on high-temperature oxidation kinetic mechanisms of both n-butanol and iso-octane were adequate [8,21,27,28]. However, there are still few work related to the oxidation kinetic mechanism of iso-octane/n-butanol blends.

Consequently, in this study, a high-temperature oxidation kinetic mechanism of iso-octane/n-butanol blends was firstly constructed, then the mechanism was validated by laminar flame speeds, ignition delay times and JSR data. Finally, detailed reaction pathway analysis was performed to point out the key factors which induce the increase of laminar flame speed of the blends compared with that of pure iso-octane.

## 2. Experimental setup

The experimental setup in this study is a constant volume combustion bomb, in cooperate with a heating system, an ignition system and an image acquisition system. The diameter and length of the cylindrical chamber is 180 mm and 210 mm, respectively. Each component is introduced according to the calculated partial pressure, then 5 min is reserved before ignition to ensure uniform mixing. Finally homogeneous mixture is ignited at the centre of the chamber and outwardly propagating spherical flame is recorded by the high speed camera. More details about the experimental equipment and procedure can be found in Refs. [29,30].

For spherical flame, flame propagation speed can be obtained from the raw flame radius ( $r_f$ ) by  $S_b = dr_f/dt$ , and flame stretch is calculated by  $k = 2S_b/r_f$ . To discard the effect of ignition energy and cylindrical confinement [31,32], the radius ranges used in extraction are restricted to 9–22 mm. In addition, the flame radius ranges are also restricted by the occurrence of cellular structure.

The extraction adopted is the nonlinear method presented by Chen et al. [33] as following:

$$S_b = S_b^0 - 2S_b^0 L_b / R_f \quad (1)$$

and the uncertainties in the experimental laminar flame speed measurements are calculated with Eq. (2) [34]:

$$\delta_{S_L} = \sqrt{(B_{S_L})^2 + \left(\frac{t_{M-1.95} S_{S_L}}{\sqrt{M}}\right)^2} \quad (2)$$

In this study, initial temperatures are set as 353 K, 393 K and 433 K, with uncertainty of 2 K, initial pressure is fixed at 0.1 MPa, and every condition is repeated 3 times to ensure its repeatability.

Numerical calculation of laminar flame speed was conducted using PREMIX codes in CHEMKIN software. The set of adaptive grid points and maximum grid points in calculation was 200 and 1000, respectively. To obtain the high-accuracy computation, the solution curvature and gradient parameters were both set to be 0.05 and the steps of calculation were >500 points in the final solution. The ignition delay times were calculated by the by Senkin codes, with an adiabatic, constant volume and zero-dimensional reactor. The simulation of JSR data was done by the PSR codes. An example of laminar flame speed calculation was also provided as a piece of [Supplementary material](#).

## 3. Mechanism construction

A comprehensive chemical kinetic mechanism for the four butanol isomers was developed by Sarathy et al. [27], and was referred to as Model I hereinafter. Model I has been proved to be valid and accurate by experimental results, including laminar flame speed, ignition delay time and intermediate species concentration, hence it was chosen as the base model for further n-butanol/iso-octane blends mechanism construction. As the flame chemistry is dominated by high-temperature oxidation reactions, so low temperature reactions were removed. Then a modified kinetic mechanism of n-butanol named Model II was obtained, which contains 284 species and 1747 elemental reactions. After the simplification process using Chem-RC developed by Ju et al. [35–37], a simplified Model II containing 98 species and 737 elemental reactions was obtained and referred to as Model III hereinafter.

Next, as for the kinetic model of iso-octane, a high-temperature oxidation mechanism developed by Chaos et al. [21] was chosen. After appropriately simplified, the Chaos mechanism called Model IV, contains 107 species and 723 elemental reactions.

**Table 1**  
Intermediate species being added into Model III.

C <sub>n</sub> (n for carbon number)	intermediate species
C <sub>8</sub>	iC <sub>8</sub> H <sub>18</sub> aC <sub>8</sub> H <sub>17</sub> bC <sub>8</sub> H <sub>17</sub> cC <sub>8</sub> H <sub>17</sub> dC <sub>8</sub> H <sub>17</sub>
C <sub>7</sub>	xC <sub>7</sub> H <sub>15</sub> yC <sub>7</sub> H <sub>15</sub> pC <sub>7</sub> H <sub>15</sub> xC <sub>7</sub> H <sub>14</sub> yC <sub>7</sub> H <sub>14</sub> oC <sub>7</sub> H <sub>14</sub> pC <sub>7</sub> H <sub>14</sub>
C <sub>6</sub>	iC <sub>6</sub> H <sub>11</sub>
C <sub>5</sub>	neoC <sub>5</sub> H <sub>11</sub>
C <sub>4</sub>	tC <sub>4</sub> H <sub>9</sub> iC <sub>4</sub> H <sub>8</sub> iC <sub>4</sub> H <sub>8</sub> iC <sub>4</sub> H <sub>7</sub> iC <sub>4</sub> H <sub>10</sub> iC <sub>3</sub> H <sub>5</sub> CHO iC <sub>4</sub> H <sub>7</sub> O iC <sub>4</sub> H <sub>7</sub> OH iC <sub>4</sub> H <sub>6</sub> OH iC <sub>3</sub> H <sub>5</sub> CO iC <sub>3</sub> H <sub>6</sub> CO tC <sub>3</sub> H <sub>6</sub> CHO iC <sub>3</sub> H <sub>5</sub> O <sub>2</sub> HCHO iC <sub>4</sub> H <sub>8</sub> OH tC <sub>3</sub> H <sub>6</sub> O <sub>2</sub> CHO tC <sub>3</sub> H <sub>6</sub> O <sub>2</sub> HCO
C <sub>3</sub>	tC <sub>3</sub> H <sub>6</sub> OH iC <sub>3</sub> H <sub>7</sub> O CH <sub>3</sub> COCH <sub>3</sub>

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