Combustion and Flame 157 (2010) 240–245

Contents lists available at ScienceDirect

Combustion and Flame

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

Ignition properties of *n*-butane and iso-butane in a rapid compression machine

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ARTICLE INFO

Article history:
Received 27 March 2009
Received in revised form 2 October 2009
Accepted 21 October 2009
Available online 14 November 2009

Keywords:
Autoignition
Butane
Simulation
Measurement

ABSTRACT

Autoignition delay times of *n*-butane and iso-butane have been measured in a Rapid Compression Machine in the temperature range 660–1010 K, at pressures varying from 14 to 36 bar and at equivalence ratios $\varphi = 1.0$ and $\varphi = 0.5$. Both butane isomers exhibit a negative-temperature-coefficient (NTC) region and, at low temperatures, two-stage ignition. At temperatures below ~900 K, the delay times for iso-butane are longer than those for the normal isomer, while above this temperature both butanes give essentially the same results. At temperatures above ~720 K the delay times of the lean mixtures are twice those for stoichiometric compositions; at $T < 720$ K, the equivalence ratio is seen to have little influence on the ignition behavior. Increasing the pressure from 15 bar to 30 bar decreases the amplitude of the NTC region, and reduces the ignition delay time for both isomers by roughly a factor of 3. In the region in which two-stage ignition is observed, 680–825 K, the duration of the first ignition stage decreases sharply in the range 680–770 K, but is essentially flat above 770 K. Good quantitative agreement is found between the measurements and calculations for *n*-butane using a comprehensive model for butane ignition, including both delay times in the two-stage region, with substantial differences being observed for iso-butane, particularly in the NTC region.

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1. Introduction

The study of the ignition properties of butane has both fundamental and practical relevance. Practically, butane is an important component in modern fuels and, due to the fuel sensitivity of engine knock [1], knowledge concerning the ignition behavior of butane is essential in the development and optimization of internal combustion engines. For example, mixtures of propane and butane (liquid petroleum gas, LPG) are an important automotive fuel. Also, while methane is the main constituent in natural gas, depending on the source it may contain significant amounts of higher hydrocarbons such as *n*-butane and iso-butane. It is known that small changes in the volume fraction of butane strongly affect the ignition properties of natural gas [2–5] and therefore may result in the occurrence of knock in automotive engines using compressed natural gas (CNG) or stationary engines used for power generation. Knowledge regarding the autoignition behavior of butane is also relevant for the performance and development of Homogeneous Charge Compression Ignition (HCCI) engines [6] and gas turbines [7,8]. From a fundamental perspective, measured autoignition delay times are used as targets for the development and verification of chemical kinetic models. Moreover, butane is the simplest fuel having a branched isomer, and that exhibits the complex combustion properties observed in larger hydrocarbons, such as cool flame appearance [9,10], negative-temperature-coefficient (NTC) behavior and two-stage autoignition [9–14]. This makes butane an interesting model system for investigating such behavior, particularly any variations in behavior between the isomers.

Several studies have been conducted to study the autoignition behavior of *n*-butane in shock tubes [15–18] and Rapid Compression Machines (RCM) [9–14]. Measurements in the RCM have been performed at temperatures between ~600 and 900 K and pressures below 18 bar. In general, the results showed two-stage ignition and NTC behavior. Although the ignition behavior of *n*-butane differs from iso-butane, only a few iso-butane ignition studies have been performed [13,17,18]. For example, the ignition properties of stoichiometric *n*-butane and iso-butane mixtures were investigated in an RCM at pressures below 9 bar and temperatures ranging from 600 to 900 K [13]. The authors observed an NTC region for *n*-butane, but no such feature was observed for iso-butane. Recently, autoignition of stoichiometric and fuel-lean *n*-butane and iso-butane mixtures were studied in a shock tube over a temperature range of 1150–1450 K and an average pressure of 1.45 atm [17]. The experimental results showed that the autoignition delay times of *n*-butane were shorter than those of iso-butane over the entire measured domain, as also seen in [18]. Investigations of iso-butane at high pressures and moderate temperatures are lacking. It is also interesting to extend current existing data on *n*-butane ignition to higher pressures, which are more relevant to engines.

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doi:10.1016/j.combustflame.2009.10.012

Here we extend the investigation of both *n*-butane and iso-butane to higher pressures more relevant for SI engines and gas turbines, and report measurements at pressures ranging from 14 to 36 bar and temperatures between 660 and 1010 K, under both stoichiometric $\varphi = 1.0$ and fuel-lean $\varphi = 0.5$ conditions. All measurements have been performed in a Rapid Compression Machine and compared with numerical simulations using a recently developed chemical mechanism including both butane isomers [19].

2. Experimental procedure

The experiments were conducted in an RCM of the same design, construction and specification reported in [20,21], used in our previous study of methane/hydrogen mixtures [22]. A creviced piston head designed for this machine [20,23] was used to preserve a homogeneous reacting core gas. The gas mixtures were compressed in ~10–20 ms to peak pressures, while the majority of the pressure rise takes place in less than 3 ms. The pressure in the combustion chamber during compression and throughout the post-compression period were measured using a Kistler 6025B piezoelectric pressure transducer with a Kistler 5010B charge amplifier. The compositions of the gas mixtures studied, expressed in mole fraction, are given in Table 1. The total fraction of the inert gases in the fuel/oxidizer mixtures is close to that of nitrogen in air, while the Ar/N_2 ratio is chosen to provide similar temperatures after compression for different equivalence ratios. To consider non-ideal effects in the RCM such as heat loss, which is necessary for accurate simulation of the results (see below), for each experiment for a given fuel/oxidizer mixture a corresponding measurement in an inert mixture was performed, where the fuel was replaced by CO_2 and the CO_2/O_2 ratio was slightly adjusted to provide the same heat capacities as in the reactive mixtures.

The gas mixtures were prepared in advance in a 10 l gas bottle and allowed to mix ~72 h to ensure homogeneity. The butane isomers used in the experiments have purity greater than 99.95%, while the rest of the gases were 99.99% pure or better. The desired gas temperature and pressure at the end of compression is controlled by varying the compression ratio and the initial pressure. Autoignition delay times for the butane/oxidizer mixtures are obtained in a range of temperatures (660–1010 K) at compressed gas pressures of 15 and 30 bar, and at equivalence ratios of $\varphi = 1.0$ and $\varphi = 0.5$. In addition, to study the pressure dependence of these mixtures, a substantial number of measurements have been performed along isotherms at 900 ± 4 K, between ~14 and 36 bar.

To avoid uncertainties regarding the actual specific volume of the core gas within the combustion chamber, the measured pre-ignition peak pressure after compression, P_c and the initial pressure, P_i, together with the initial temperature T_i, are used to calculate the peak temperature after compression, T_c of the adiabatic core gas assuming isentropic compression. The state of the gas can be determined by solving

$$S(T_i, P_i) = S(T_c, P_c), \tag{1}$$

Table 1
Composition of mixtures (mole fractions).

No.	φ	n-C_4H_{10}	iso-C_4H_{10}	O_2	N_2	Ar
A	1	0.0311	0	0.194	0.549	0.226
B	0.5	0.0165	0	0.206	0.400	0.378
C	1	0	0.0311	0.194	0.549	0.226
D	0.5	0	0.0165	0.206	0.400	0.378
E	1	0.0075	0.0224	0.194	0.55	0.226
F	1	0.0149	0.0149	0.194	0.55	0.226
G	1	0.0224	0.0075	0.194	0.55	0.226

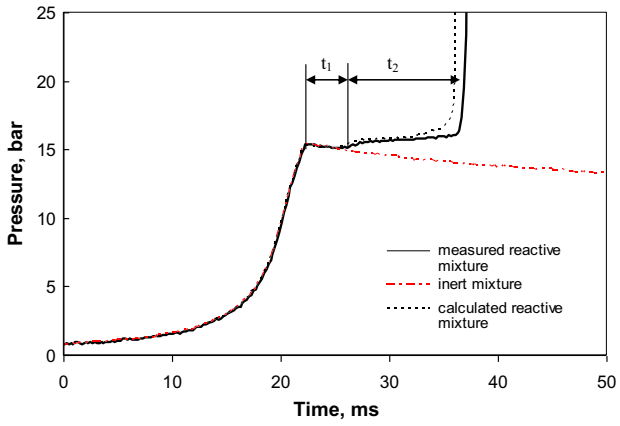

Fig. 1. Pressure traces for mixtures at $T = 800$ K; pressure measured in reactive mixture A (solid line), pressure measured in the inert mixture (red dashed line) and calculated reacting pressure trace (dotted line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

where S is the entropy of the mixture. Alternatively, as done here, one can also use

$$\ln\left(\frac{P_c}{P_i}\right) = \int_{T_i}^{T_c} \frac{\gamma}{\gamma - 1} d\ln T, \tag{2}$$

where $\gamma(T)$ is the ratio of the temperature dependent heat capacities of the mixture. The temperature T_c can be obtained iteratively from Eq. (2), where the heat capacities used in this study were taken from [19]. For experiments under identical conditions the reproducibility of the measured ignition delay is ~5%. For the data taken along an isotherm, the variation in temperature at the end of compression (±4 K), caused primarily by the reproducibility in the setting of the compression ratio, yields a scatter in the measured delay times of 10–20% [22].

3. Simulation procedure

For meaningful comparison between measurements and numerical simulations it is necessary to account for deviations from ideal behavior, such as heat loss, that occur during the measurements in the simulations [20,22–27]. Often for this purpose the specific volume of the assumed adiabatic core is used as input into the simulations. One method derives the specific volume based on the measured pressure trace in an inert mixture having the same heat capacity, initial temperature and initial pressure as that in the reactive mixture under investigation [22,24–27]. Deriving the temperature of the adiabatic core from the relation shown in Eq. (2), the profile of specific volume, $V(t)$, can be obtained from the adiabatic relations between pressure and volume, i.e., $V(t)/V_i = (P(t)/P_i)^{1/\gamma}$. We follow this method here, and obtained specific volumes from measurements on an equivalent inert mixture for each set of conditions studied, which were subsequently used as input in simulations[1] using the zero-dimensional SENKIN code [28]. The comprehensive chemical mechanism [19] used in the simulations is comprised of 1580 reactions and 289 species. It is beyond the scope of the discussion of our experimental results to analyze or comment on the chemical mechanisms used here; for details regarding the mechanism, including kinetic data, we refer to the authors [19]. The computations presented are solely intended to illustrate the degree to which recent models can reproduce the experimental trends.

Fig. 1 shows the experimental pressure traces for both a reactive (mixture A, compression to ~15 bar and 800 K) and an inert

[1] Note: the data are available upon request for simulations.

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