

An Experimental Study of Butene Isomers and 1,3-Butadiene Ignition Delay Times at Elevated Pressures

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Abstract

In this study, rapid compression machine (RCM) and shock tube (ST) ignition delay time measurements have been made for three butene isomers (*iso*-butene, 1-butene and *trans*-2-butene) for fuel/air mixtures at equivalence ratios of 0.5, 1.0, and 2.0 over a wide temperature range, and across engine relevant pressures, ranging from 10 to 50 atm. Some ignition delay time measurements of 1,3-butadiene have also been obtained at both low and elevated pressures. The results for the butene isomers show that, for several pressures and equivalence ratios, the ST and RCM results are in excellent agreement at overlapping temperatures and are very complementary to one another. A negative temperature coefficient (NTC) behaviour was not observed for any of the butene isomers at any of the conditions studied. At relatively low temperature conditions (≤ 1000 K), ignition delay time decreases with increasing equivalence ratio, while at relatively high temperature conditions (≥ 1000 K), there appears to be no dependence on equivalence ratio under the conditions investigated. It was found that reactivity increases with increasing pressure for all fuels. 1-Butene is the most reactive, followed by *trans*-2-butene, with *iso*-butene being the slowest to ignite at the same conditions of temperature and pressure. As to 1,3-butadiene ignition, we can see that reactivity increases with pressure at all equivalence ratios and at all levels of dilution presented. As the pressure increases, the relative concentration of the reactants increases, thereby increasing the overall reactivity. These experimental results will be used to validate detailed chemical kinetic models for all these fuels studied.

Introduction

The isomeric structure of a fuel can fundamentally affect its combustion chemistry and consequently the nature of its practical applications. For example, the research octane numbers of the heptane isomers vary from 0 for *n*-heptane to 112 for 2,2,3-trimethylbutane [1]. Butene (C₄H₈), being the smallest alkene with isomeric structures, is a common component in many practical fuels, particularly liquid petroleum gas. Compared to larger alkenes, it has the essential features of the double bond variation with the smallest number of isomers, and its four isomers are all gaseous at room temperature and at moderate pressures. Experimental studies have been performed on various aspects of butene combustion, including pyrolysis and oxidation, measurements of ignition delay times, speciation, flame speed, ignition temperature, etc., shown in Tables 1–3. However, few studied have been specifically concerned with the effects of isomeric fuel structures. In addition, while kinetic models have been developed for the combustion process of specific butene isomers, only a few have been reported for all of the butene isomers. This is possibly due to the paucity of experimental studies of isomeric effects at identical conditions.

Most recently, Schenk *et al.* [2] studied premixed low-pressure (40 mbar) flat argon-diluted (25%) flames of the three butene isomers (1-, *trans*-2-, and *iso*-butene) under fuel-rich ($\Phi = 1.7$) conditions. It was the first detailed flame study of butene isomers, performed under fuel-rich conditions. The isomer-specific species information and the quantitative mole fraction profiles of more than 30 stable and radical species measured by

a newly developed analytical combination of high-resolution *in situ* molecular-beam mass spectrometry (MBMS) and *in situ* gas chromatography (GC) were used to validate and improve the subset of C₄ kinetics in a general hydrocarbon oxidation mechanism based on the work of Hoyermann *et al.* [3]. In addition, Zhao *et al.* [4] developed a high temperature kinetic model for the four butene isomers (1-, *trans*-2-, *cis*-2- and *iso*-butene) based on validation against the laminar flame speeds and non-premixed counterflow ignition temperatures at pressures of 2, 5 and 10 atm. Furthermore, the critical reaction paths for butene isomer oxidation during ignition, particularly the allylic H-atom abstraction by OH radical with isomeric butenes, the OH radical induced oxidation reactions of butenes, and reactions between butenyl radicals and HO₂/O₂, etc., were systematically considered with updated rate coefficients from *ab initio* calculations and kinetic theories.

As the simplest conjugated hydrocarbon, 1,3-butadiene (1,3-C₄H₆) can also provide a first step towards understanding the role of complex alkenes in combustion and, in particular, an understanding of the contribution of 1,3-butadiene towards soot formation. For example, in diesel engines, practical hydrocarbon fuels do not actually contain 1,3-butadiene, but it is a stable intermediate species which is produced in large quantities during the combustion of olefins (which constitute several percent in gasoline) [5, 6]. It is the oxidation of 1,3-butadiene that can lead to the formation of benzene, which is central to the formation of soot [5]. Literature data of 1,3-butadiene oxidation is summarized in Table 4.

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Most recently, Laskin *et al.* [7] examined high-temperature kinetics of 1,3-butadiene oxidation with detailed kinetic modeling. To facilitate model validation, flow reactor experiments were carried out for 1,3-butadiene pyrolysis and oxidation over the temperature range 1035–1185 K and at atmospheric pressure, extending the literature data. Libby *et al.* [8] presented hydroxyl (OH) radical concentration-time histories and ignition delay times measured in dilute 1,3-butadiene/O₂/argon mixtures after reflected shock waves. Temperature ranged from 1230 K to 1890 K at pressures from 1.5–7.5 atm with fuel concentrations from 250–5000 ppm at ϕ in the range 0.25–2.0. It was the first shock tube study of 1,3-butadiene oxidation that included quantitative measurements of a radical species-time histories. Moreover, experimental results were compared to the predictions of four different 1,3-butadiene oxidation mechanisms in the literature. Zheng *et al.* [9] investigated the ignition temperatures of

nitrogen-diluted 1,3-butadiene by heated air in counterflow at pressures up to 5 atm and pressure-weighted strain rates from 100 to 250 s⁻¹. Experimental data were compared with computational results using the mechanism of Laskin *et al.* [7] which was then simplified to skeletal and reduced mechanisms.

Despite their importance, there is a lack of experimental data available in the literature for both the butene isomers, and 1,3-butadiene at low and intermediate temperatures (700–1200 K), and at high pressures (≥ 10 atm). From this point of view, ignition delay time measurements have been made for three butene isomers (*iso*-, 1- and *trans*-2-butene) for fuel/air mixtures at equivalence ratios of 0.5, 1.0, and 2.0 in a wide temperature range, and across engine relevant pressures, ranging from 10 to 50 atm. Ignition delay time measurements of 1,3-butadiene have also been made at both low and elevated pressures.

Table 1. List of Experimental Data of *Iso*-butene at High-Temperature.

No.	Reactor	Φ	Diluent / %	T / K	p / atm	References
1	Shock Tube	0.1, 0.2, 0.4, 0.5, 0.8, 1.0, 2.0, 4.0	80.8–98.8 (Ar)	1200–2000	2.2, 3.5, 3.6, 4.4, 4.5, 4.6	Curran [29]
2	Shock Tube	1.0, 2.0, 3.0	74.45–98.5 (Ar)	1230–1930	9.5–10.5	Bauge <i>et al.</i> [19]
3	Shock Tube	0.125, 0.5, 0.6, 1.0, 2.0, ∞	93.0–99.0 (Ar)	1000–1800	1.0–2.7	Yasunaga <i>et al.</i> [14]
4	Shock Tube	∞	-	1055–1325	2.92–4.0	Bradley <i>et al.</i> [20]
5	Shock Tube	-	99.0–99.25 (Ar)	1000–1180	2.5–3.0	Tsang <i>et al.</i> [21]
6	Shock Tube	∞	90.0–98.0 (Kr)	900–2300	7–400 / torr	Santhanam <i>et al.</i> [26]
7	JSR	3.0, 6.0	83.3–86.95 (He)	833–913	1.0	Bauge <i>et al.</i> [3]
8	JSR	0.2, 0.5, 1.0, 2.0	95.35–99.4	790–1240	1.0	Dagaut <i>et al.</i> [22]
9	Flow Reactor	∞	96.0 (Ar)	900–1900	3–12 / torr	Zhang <i>et al.</i> [27]
10	Flow Reactor	-	-	1080	1.0	Brezinsky <i>et al.</i> [28]
11	Flame Burner	1.7	25.0 (Ar)	2046	0.04	Schenk <i>et al.</i> [2]
12	Flame Burner	0.225	9.8 (Ar)	1720	0.04	Dias <i>et al.</i> [30]
13	Counterflow	0.7–1.7	74.6–77.1	2321	1.0, 2.0, 5.0, 10	Davis <i>et al.</i> [31]
14	Counterflow	-	-	1000–1300	1.0–5.0	Zhao <i>et al.</i> [4]

Table 2. List of Experimental Data of 1-Butene at High-Temperature.

No.	Reactor	Φ	Diluent / %	T / K	p / atm	References
1	Shock Tube	0.5, 1.0, 2.0	86.0–96.0 (Ar)	1200–1670	6.6–8.9	Heyberger <i>et al.</i> [15]
2	JSR	0.4, 4.0	99.9	900–1200	1.5–10	Heyberger <i>et al.</i> [15]
3	JSR	0.15, 1.0, 4.0	90.0–93.85	900–1200	1.0–10.0	Chakir <i>et al.</i> [16]
4	Flow Reactor	∞	96.0 (Ar)	900–1900	3–12 / torr	Zhang <i>et al.</i> [27]
5	Flame Burner	1.7	25.0 (Ar)	2204	0.04	Schenk <i>et al.</i> [2]
6	Counterflow	0.7–1.7	74.6–77.1	2329	1.0, 2.0, 5.0, 10	Davis <i>et al.</i> [31]
7	Counterflow	-	-	1000–1300	1.0–5.0	Zhao <i>et al.</i> [4]

Table 3. List of Experimental Data of *Trans*-2-butene at High-Temperature.

No.	Reactor	Φ	Diluent / %	T / K	p / atm	References
1	JSR	0.5, 1.0, 2.0	94.0	900–1450	1.0	Fenard <i>et al.</i> [17]
2	Combustion bomb	0.8–1.4	75.3–76.8	300	1.0	Fenard <i>et al.</i> [17]
3	Flow Reactor	∞	96.0 (Ar)	900–1900	3–12 / torr	Zhang <i>et al.</i> [27]
4	Flame Burner	1.7	25.0 (Ar)	2218	0.04	Schenk <i>et al.</i> [2]
5	Counterflow	0.7–1.7	74.6–77.1	-	1.0, 2.0, 5.0, 10	Zhao <i>et al.</i> [4]
6	Counterflow	-	-	1000–1300	1.0–5.0	Zhao <i>et al.</i> [4]

Table 4. List of Experimental Data of 1,3-Butadiene at High-Temperature.

No.	Reactor	Φ	Diluent	T / K	p / atm	References
1	Shock Tube	0.25, 0.5, 1.0	96.75–99.425 (Ar)	1230–1890	1.7, 3.8	Libby <i>et al.</i> [8]
2	Shock Tube	0.69, 1.38	85.0–95.0 (Ar)	1200–1700	8.5–10	Fournet <i>et al.</i> [23]
3	Shock Tube	∞	99.825 (Ar)	1200–1800	6.5	Colket <i>et al.</i> [24]
4	Shock Tube	∞	99.5 (Ar)	1200–1800	1.4–2.2	Hidaka <i>et al.</i> [25]
5	Flow Reactor	0.55, 1.0, 1.62, 1.63, 4.7, ∞	98.46–99.74	1035–1185	1.0	Laskin <i>et al.</i> [7]
6	Flow Reactor	1.18, 1.65	99.231–99.38	1125	1.0	Brezinsky <i>et al.</i> [28]
7	Counterflow	∞	94.1	1020–1220	1.0–5.0	Zheng <i>et al.</i> [9]
8	Counterflow	0.7–1.7	-	2381	1.0	Davis <i>et al.</i> [31]

Experiments

The high-pressure shock tube (HPST) used in this study consists of a stainless steel tube of 8.76 m in length, with an internal diameter of 6.35 cm. A 3 cm long double-diaphragm section divides the shock tube into a 3 m long driver section and a 5.73 m driven section. The diagnostic system involves seven pressure transducers, where the velocity of the incident shock wave was measured at six locations separated by known distances with the shock velocity extrapolated to the endwall. The incident shock velocity at the endwall was used to calculate the temperature and pressure of the mixtures behind the reflected shock wave using the equilibrium program Gaseq [10]. The ignition delay time was defined as the interval between the rise in pressure due to the arrival of the shock wave at the endwall and the maximum rate of rise of the pressure signal, Fig. 1. Estimated uncertainty limits of the measurements are ± 15 K in reflected shock temperature, T_5 , $\pm 15\%$ in ignition delay time, τ , and $\pm 10\%$ in mixture concentration.

The RCM used in this study is a clone of the original NUI Galway machine, which is characteristically different to most other RCMs in that it has a twin-opposed piston configuration, as described previously [11], resulting in a fast compression time of approximately 16 ms. Additionally, creviced piston heads are used to improve the post compression

temperature distribution in the combustion chamber [12]. Pressure–time profiles are measured using a pressure transducer (Kistler 6045A). The ignition delay time was defined as the time from the peak pressure near the end of compression to the maximum rate of pressure rise during ignition. In general, it was found that the ignition delay times were reproducible to within 15% of one other at each compressed temperature. The compressed gas pressure was measured using two horizontal cursors. The time for compression is fast, ≈ 16 ms, with most of the rapid rise in pressure and temperature taking place in the last 2–3 ms of compression; therefore heat losses during compression are small. For a period following compression, the gases experience a high degree of heat loss owing to the swirl experienced and the high temperature of the gas within the chamber. Heat losses continue from the core gas during the constant volume period. For this reason, non-reactive experiments are taken to account for these heat losses in simulations of the RCM ignition experiments. These non-reactive experiments replace the oxygen content with inert nitrogen. A typical pressure–time trace obtained in the rapid compression machine is shown in Fig. 2.

Detailed experimental data of three butene isomers (1-, *iso*- and *trans*-2-butene) were obtained in NUI Galway to fill the validation matrix, Tables 5–7. Some experimental data of 1,3-butadiene were obtained in NUI Galway to fill the validation matrix, Table 8.

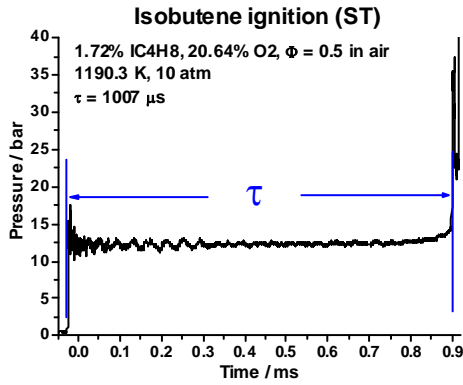


Figure 1. Typical pressure trace of *iso*-butene ignition delay time measurement in the HPST.

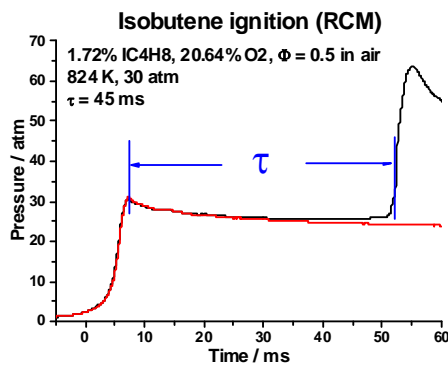


Figure 2. Typical pressure trace of *iso*-butene ignition delay time measurement in the RCM.

Table 5. Molar % composition of 1-butene mixtures.

No.	1- C ₄ H ₈	O ₂	Diluent	ϕ	p5 atm	Facility
1	1.72	20.64	77.64	0.5	10	ST
2	1.72	20.64	77.64	0.5	30	ST
3	1.72	20.64	77.64	0.5	50	ST
4	3.38	20.29	76.33	1.0	10	ST
5	3.38	20.29	76.33	1.0	30	ST
6	3.38	20.29	76.33	1.0	50	ST
7	6.54	19.63	73.83	2.0	10	ST
8	6.54	19.63	73.83	2.0	30	ST
9	6.54	19.63	73.83	2.0	50	ST

Table 8. Molar % composition of 1,3-butadiene mixtures.

No.	1,3- C ₄ H ₆	O ₂	Diluent	ϕ	p5 / atm	Facility
1	1.0	11.0	88.00	0.5	2	ST
2	1.0	5.5	93.50	1.0	2	ST
3	3.68	20.23	76.09	1.0	20	ST
4	3.68	20.23	76.09	1.0	40	ST
5	3.68	20.23	76.09	1.0	20	RCM
6	3.68	20.23	76.09	1.0	30	RCM

Table 6. Molar % composition of *iso*-butene mixtures.

No.	<i>iso</i> - C ₄ H ₈	O ₂	Diluent	ϕ	p5 / atm	Facility
1	1.04	20.78	78.18	0.3	10	ST
2	1.04	20.78	78.18	0.3	30	ST
3	1.04	20.78	78.18	0.3	50	ST
4	1.04	20.78	78.18	0.3	10	RCM
5	1.04	20.78	78.18	0.3	30	RCM
6	1.04	20.78	78.18	0.3	50	RCM
7	1.72	20.64	77.64	0.5	10	ST
8	1.72	20.64	77.64	0.5	30	ST
9	1.72	20.64	77.64	0.5	50	ST
10	1.72	20.64	77.64	0.5	10	RCM
11	1.72	20.64	77.64	0.5	30	RCM
12	1.72	20.64	77.64	0.5	50	RCM
13	3.38	20.29	76.33	1.0	10	ST
14	3.38	20.29	76.33	1.0	30	ST
15	3.38	20.29	76.33	1.0	50	ST
16	3.38	20.29	76.33	1.0	10	RCM
17	3.38	20.29	76.33	1.0	30	RCM
18	3.38	20.29	76.33	1.0	50	RCM
19	6.54	19.63	73.83	2.0	10	ST
20	6.54	19.63	73.83	2.0	30	ST
21	6.54	19.63	73.83	2.0	50	ST
22	6.54	19.63	73.83	2.0	10	RCM
23	6.54	19.63	73.83	2.0	30	RCM

Table 7. Molar % composition *trans*-2-butene mixtures.

No.	<i>trans</i> - 2- C ₄ H ₈	O ₂	Diluent	ϕ	p5 / atm	Facility
1	1.72	20.64	77.64	0.5	10	ST
2	1.72	20.64	77.64	0.5	30	ST
3	1.72	20.64	77.64	0.5	50	ST
4	3.38	20.29	76.33	1.0	10	ST
5	3.38	20.29	76.33	1.0	30	ST
6	3.38	20.29	76.33	1.0	50	ST
7	6.54	19.63	73.83	2.0	10	ST
8	6.54	19.63	73.83	2.0	30	ST
9	6.54	19.63	73.83	2.0	50	ST

Results and Discussions

As regards the fuels studied in this paper, for several pressures and equivalence ratios, the ST and RCM results are in excellent agreement. NTC behaviour was not observed at any of the conditions studied.

- *Butene isomers*

The effect of pressure on ignition delay times for three butene isomers (1-, *iso*- and *trans*-2-butene) was studied at four equivalence ratios in air (0.3, 0.5, 1.0 and 2.0). Ignition delay times of *iso*-butene oxidation versus inverse temperature at an equivalence ratio of 1.0 and at pressures of approximately 10, 30 and 50 atm are shown in Fig. 3. At these conditions, reactivity increases with increasing pressure, that is, shorter ignition delay times were measured for higher pressures. The same trends are observed for *iso*-butene/air mixtures at equivalence ratios of 0.3, 0.5 and 2.0 at the same reflected shock pressures. Meanwhile, the same trends are observed for both 1-butene/air and *trans*-2-butene/air mixtures at equivalence ratios of 0.5, 1.0 and 2.0, at the same reflected shock pressures as well. This indicates a consistent trend of reactivity of butene isomers with pressure throughout this study. These results are typical of the effect of pressure on ignition delay time [13].

The effect of equivalence ratio on ignition delay times for three butene isomers (1-, *iso*- and *trans*-2-butene) was determined for four fuel/air mixture compositions at 10, 30 and 50 atm. The effect of equivalence ratio on *iso*-butene ignition at a pressure of 30 atm at the four equivalence ratios studied (0.3, 0.5, 1.0 and 2.0) is shown in Fig. 4. At relatively low temperature conditions (≤ 1000 K), ignition delay time decreases with increasing equivalence ratio, while at relatively high temperature conditions (≥ 1000 K), there appears to be very little dependence on equivalence ratio.

The effect of isomeric structure on ignition delay times for three butene isomers (1-, *iso*- and *trans*-2-butene) was determined for four fuel/air mixture compositions (0.3, 0.5, 1.0 and 2.0) at pressures of 10, 30 and 50 atm. The effect of isomeric structure for three butene isomers ignition at an equivalence ratio of 1.0 at a pressure of 10 atm is shown in Fig. 5. 1-Butene is the fastest to ignite, followed by *trans*-2-butene, with *iso*-butene being the slowest.

- *1,3-butadiene*

The effect of equivalence ratio on ignition delay times for 1,3-butadiene dilute mixtures at low pressure was determined, Fig. 6. The ignition delay times at $\phi = 0.5$ are shorter than those of $\phi = 1.0$. This is simply because of the higher concentration of reactants in $\phi = 0.5$ mixture.

The effect of pressure on ignition delay times for 1,3-butadiene was studied at an equivalence ratio of 1.0 at pressures of 20, 30 and 40 atm, Fig. 7. We can see that reactivity increases with increasing pressure. As the pressure increases, the relative concentration of the reactants increases, thereby increasing the overall rate of reactivity.

More experimental conditions will be studied to cover a wide temperature range at equivalence ratios of 0.3, 0.5, 1.0 and 2.0 at pressures of 10, 20 and 40 atm in the near future.

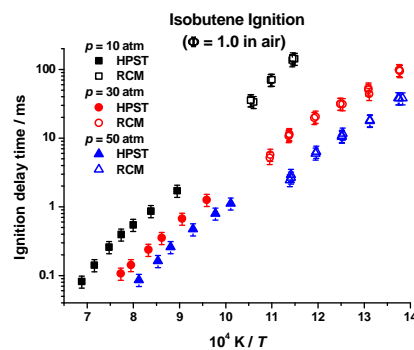


Figure 3. Effect of varying pressure on *iso*-butene reactivity.

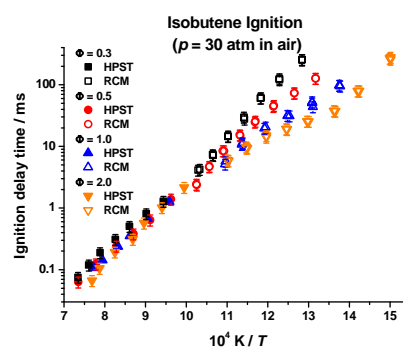


Figure 4. Effect of varying equivalence ratio on *iso*-butene reactivity.

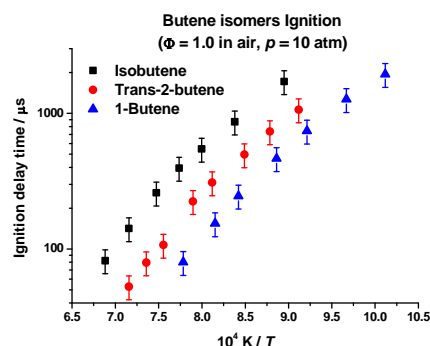


Figure 5. Effect of varying isomeric structure on *iso*-butene, *trans*-2-butene and 1-butene reactivity.

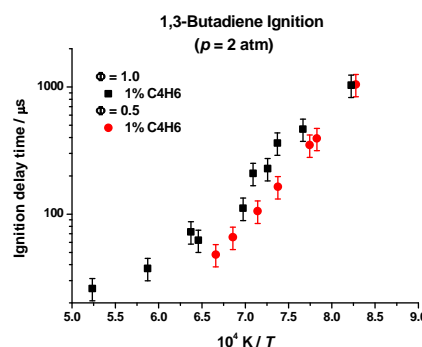


Figure 6. Effect of varying equivalence ratio on 1,3-butadiene reactivity.

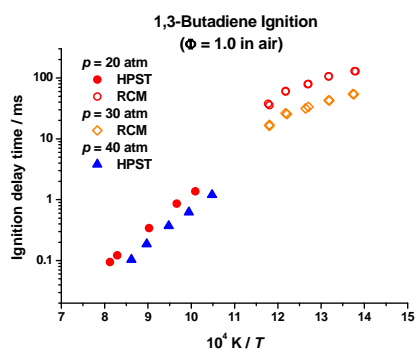


Figure 7. Effect of varying pressure on 1,3-butadiene reactivity.

Conclusions

This work represents the first comprehensive ignition delay study of three butene isomers and 1,3-butadiene oxidation at elevated pressures in a high-pressure shock tube and a rapid compression machine over a wide range of pressures, temperatures and equivalence ratios. Ignition delay times were measured at temperatures in the range 650–1450 K, at pressures of 2, 10, 30 and 50 atm and at equivalence ratios of 0.3, 0.5, 1.0 and 2.0.

It was found that an increase in reflected shock pressure resulted in shorter ignition delay times (higher reactivity) for all equivalence ratios investigated, which is typical of the influence of pressure on fuel reactivity. The effect of equivalence ratio on ignition delay times depended on the temperature of the experiment, where all mixtures had similar reactivity at higher temperatures and fuel-rich mixtures were most reactive at lower temperatures. As to the effect of isomeric structure on ignition delay times for three butene isomers, 1-Butene is the fastest to ignite, followed by *trans*-2-butene, with *iso*-butene being the slowest. These experimental results will be used to validate detailed chemical kinetic models for all these fuels.

Acknowledgements

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