



Autoignition of methyl butanoate under engine relevant conditions



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ABSTRACT

This study reports the autoignition delay times of methyl butanoate in argon–air (i.e. $\text{Ar}/\text{O}_2 = 3.76$ by mole) mixtures under thermodynamic conditions relevant to compression ignition engines, using a rapid compression machine (RCM). The ignition delay times were obtained for the compressed temperature range of 833–1112 K and compressed pressures corresponding to 15, 30, 45, and 75 bar. In addition, the effect of fuel mole fraction on ignition delay times were experimentally studied by covering equivalence ratios corresponding to 0.25, 0.5, and 1.0 under realistic fuel loadings without additional dilution. For the range of conditions investigated, the ignition delay times exhibit an Arrhenius dependence on temperature and an inverse relationship with the compressed pressure. No evidence of two-stage ignition was observed in the current experiments, nor was a negative temperature coefficient trend seen in the ignition delay times. The experimental results were compared to zero-dimensional simulations taking into account the full compression stroke and the heat loss characteristics of the RCM, using chemical kinetic models reported in the literature. The literature models were found to predict significantly higher reactivity when compared to the current experiments. Chemical kinetic analysis was then conducted to identify the reactions responsible for the mismatch between the experiments and the simulated results. Key reactions that could help obtain a better match between the experimental and simulated results were identified using both brute-force and global sensitivity analyses. In view of the large uncertainties associated with the low-temperature chemistry of methyl butanoate, further studies are needed to update the kinetic parameters of the key reactions in order to improve the model comprehensiveness.

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1. Introduction

The proportion of renewable fuels used for the transportation sector is projected to be approximately 14% of the marketed renewable energy consumption by the year 2020 [1]. Combustion in engines is the predominant mode of obtaining energy from biofuels for the purpose of transportation. One of the important chemical compound classes that constitute biodiesel is methyl esters [2]. It is therefore of fundamental and practical significance to develop a basic understanding of the combustion properties of methyl esters. Of particular interest is the autoignition response, which is the fundamental basis for classification of diesel fuels in terms of their cetane numbers. The ability to predict both the global combustion properties and the detailed species evolutions during pyrolysis/oxidation of methyl esters is essential to their efficient and clean utilization in internal combustion engines. The development of predictive capabilities requires both computational and

experimental efforts. An important component of the computational efforts is the availability of a detailed reaction mechanism describing the sequence of elementary reactions that model the fuel decomposition and oxidation. The development of a comprehensive reaction mechanism can be greatly aided by fundamental experimental data derived from various complementary, well-characterized laboratory experiments covering a wide range of thermophysical conditions. Such fundamental combustion experiments provide a reliable test bed for mechanism validation.

As an experimental effort in supporting the development of detailed reaction mechanisms of methyl esters, this work reports experimental data on the autoignition delay times of methyl butanoate under thermodynamic conditions that are of relevance to engine combustion. Methyl butanoate belongs to the class of compounds that occur in biodiesel. It has been used as a biodiesel surrogate component to further the understanding of methyl ester combustion kinetics [3–10]. It is well established that chemical kinetic models have a hierarchical structure in terms of carbon numbers [11]. Therefore, methyl butanoate (and lower methyl esters) oxidation kinetics need to be fully understood as a part of the development of kinetic schemes for real biodiesel. In addition

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Table 1
Ignition delays for methyl butanoate in argon–oxygen mixtures.

Fuel	O ₂	Ar	ϕ	T_c (K)	P_c (bar)	τ (ms)	$\pm\sigma_\tau$ (ms)
Mole percentage (%)							
0.80	20.84	78.36	0.25	966	15	117.4	3.6
0.80	20.84	78.36	0.25	974	15	53.0	1.35
0.80	20.84	78.36	0.25	1007	15	22.2	1.51
0.80	20.84	78.36	0.25	1031	15	11.2	0.47
0.80	20.84	78.36	0.25	1093	15	3.2	0.07
0.80	20.84	78.36	0.25	1112	15	1.8	0.13
0.80	20.84	78.36	0.25	900	30	83.2	3.97
0.80	20.84	78.36	0.25	909	30	48.8	1.46
0.80	20.84	78.36	0.25	926	30	38.9	0.50
0.80	20.84	78.36	0.25	938	30	27.2	1.04
0.80	20.84	78.36	0.25	959	30	14.5	0.82
0.80	20.84	78.36	0.25	986	30	7.5	0.23
0.80	20.84	78.36	0.25	1016	30	4.0	0.14
0.80	20.84	78.36	0.25	1053	30	1.5	0.13
0.80	20.84	78.36	0.25	917	45	27.3	0.55
0.80	20.84	78.36	0.25	932	45	17.8	0.60
0.80	20.84	78.36	0.25	947	45	12.5	0.63
0.80	20.84	78.36	0.25	956	45	7.5	0.49
0.80	20.84	78.36	0.25	983	45	4.1	0.33
0.80	20.84	78.36	0.25	1008	45	2.1	0.99
0.80	20.84	78.36	0.25	883	75	34.5	1.71
0.80	20.84	78.36	0.25	912	75	15.8	0.47
0.80	20.84	78.36	0.25	923	75	12.1	0.95
0.80	20.84	78.36	0.25	936	75	6.8	0.30
0.80	20.84	78.36	0.25	950	75	5.3	0.76
0.80	20.84	78.36	0.25	969	75	4.0	0.35
1.59	20.67	77.74	0.50	938	15	63.5	2.25
1.59	20.67	77.74	0.50	958	15	28.1	1.47
1.59	20.67	77.74	0.50	972	15	16.2	0.59
1.59	20.67	77.74	0.50	995	15	10.4	0.84
1.59	20.67	77.74	0.50	1019	15	7.2	0.52
1.59	20.67	77.74	0.50	872	30	64.3	1.76
1.59	20.67	77.74	0.50	883	30	46.6	1.76
1.59	20.67	77.74	0.50	891	30	34.8	1.16
1.59	20.67	77.74	0.50	904	30	23.4	0.85
1.59	20.67	77.74	0.50	915	30	15.2	0.68
1.59	20.67	77.74	0.50	928	30	12.2	0.83
1.59	20.67	77.74	0.50	940	30	9.8	0.61
1.59	20.67	77.74	0.50	950	30	7.4	0.32
1.59	20.67	77.74	0.50	965	30	5.5	0.37
1.59	20.67	77.74	0.50	1001	30	2.4	0.28
3.13	20.35	76.52	1.00	881	15	76.4	1.20
3.13	20.35	76.52	1.00	896	15	41.8	0.88
3.13	20.35	76.52	1.00	927	15	27.9	2.07
3.13	20.35	76.52	1.00	937	15	17.5	0.85
3.13	20.35	76.52	1.00	954	15	10.8	0.75
3.13	20.35	76.52	1.00	975	15	4.9	0.43
3.13	20.35	76.52	1.00	990	15	3.9	0.62
3.13	20.35	76.52	1.00	833	30	57.7	2.32
3.13	20.35	76.52	1.00	847	30	37.4	1.13
3.13	20.35	76.52	1.00	861	30	21.6	0.61
3.13	20.35	76.52	1.00	871	30	12.6	1.06
3.13	20.35	76.52	1.00	881	30	10.0	0.66
3.13	20.35	76.52	1.00	896	30	5.7	0.47
3.13	20.35	76.52	1.00	908	30	4.4	0.46

to providing experimental autoignition results under previously unreported conditions, we compared the newly-obtained experimental results to computational predictions using various reaction mechanisms reported in the literature. Both a global sensitivity analysis and a brute-force one-at-a-time sensitivity analysis were further performed on the computational results to identify the reaction steps influencing the computed ignition delay times. In the following, we highlight the experimental and modeling studies on methyl butanoate reported in the literature.

The autoignition of methyl butanoate has been previously studied using a rapid compression machine (RCM) by Dooley et al. [12] for equivalence ratios in the range of $\phi = 0.33 - 1.0$, pressures of 10, 15, 20, and 40 atm, and a temperature span of 640–949 K. The work of Dooley et al. [12] varied the proportion of oxygen in the oxygen-inert mixture to obtain the results for $\phi =$

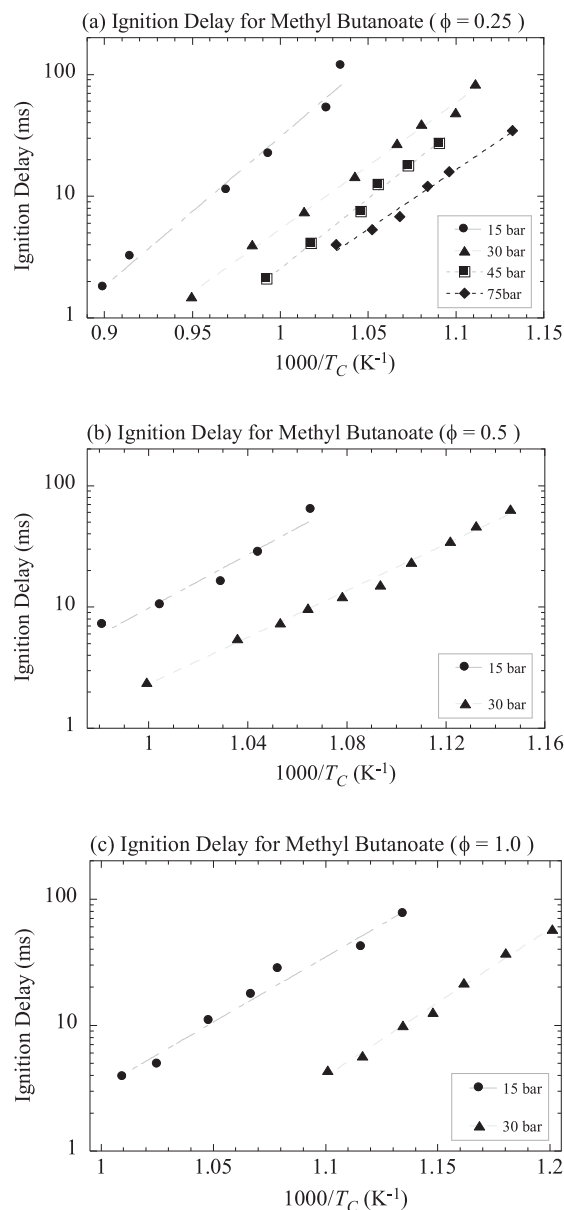


Fig. 1. Ignition delay times as a function of compressed temperature (T_c), with compressed pressure (P_c) as a parameter for (a) $\phi = 0.25$, (b) $\phi = 0.5$, and (c) $\phi = 1.0$.

0.33. The low-temperature autoignition of stoichiometric methyl butanoate mixtures has also been previously reported by HadjAli et al. [13] for a temperature span of 815 ± 20 K and pressures between 15.5 and 20.5 bar, using an RCM. In addition, Walton et al. [14] have reported the ignition delay times for methyl butanoate for equivalence ratios of 0.3–0.4, a pressure range of 4.7–19.6 bar, and temperatures varying from 935 K to 1117 K, using a rapid compression facility. In Walton et al. [14], the total inert-to-oxygen molar ratio was kept ~ 3.76 , while the inert gases (Ar or O₂) were varied.

Compared to the literature RCM studies, the current work explores an equivalence ratio that is leaner and covers a range of $\phi = 0.25 - 1.0$. This work has a fixed inert-to-oxygen proportion corresponding to Ar/O₂ molar ratio of 3.76 for all equivalence ratios. Further, the current RCM study extends the compressed pressures up to 75 bar and the compressed temperatures up to 1112 K.

Autoignition of methyl butanoate has also been studied in the shock tube apparatus. Akih-Kumgeh and Bergthorson [15] studied

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