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Brief Communications

Autoignition of methylcyclohexane at elevated pressures

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ABSTRACT

Autoignition of methylcyclohexane (MCH) is investigated in a rapid compression machine (RCM). Experiments are conducted for homogeneous MCH/O₂/N₂/Ar mixtures with equivalence ratios varying from 0.5 to 1.5, at compressed charge pressures of 15.1 and 25.5 bar, and over a compressed gas temperature range of 680–905 K. In the RCM experiments, the mole percentage of MCH is kept constant at 1.047%, while the equivalence ratio is varied through variation in oxygen mole percentage. Ignition delay measurements demonstrate the features of two-stage ignition characteristics and strong negative temperature coefficient (NTC) behavior. The NTC behavior is also noted to shift to higher temperatures at higher pressures and for oxygen-rich mixtures. In addition, both the first-stage and total ignition delays show significant dependence on oxygen mole fraction. Furthermore, the current ignition delay measurements provide additional benchmark data for the validation of the oxidation kinetics of MCH. Comparison of the experimental ignition delays with the simulated results using an available detailed kinetic mechanism is conducted and discussed.

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1. Introduction

Although cycloalkanes constitute a significant fraction in diesel and jet fuels, kinetic studies on cyclic alkanes are meager. Methylcyclohexane (MCH) is recognized as a candidate cycloalkane for surrogate formulation, and is also considered as the starting point for the development of kinetic mechanisms of other cycloalkanes. Previous investigations on MCH combustion include low pressure pyrolysis [1], pyrolysis and oxidation of MCH and the MCH/toluene blends in a turbulent plug flow reactor [2], laminar diffusion flame experiments [3], high temperature shock tube experiments and modeling [4], experiments and modeling in a rapid compression machine (RCM) [5], and shock tube ignition delay measurements at elevated pressures [6,7]. In an attempt to develop a comprehensive mechanism for MCH, Pitz et al. [5] developed a low temperature mechanism for MCH and merged it with a recent high temperature mechanism from [4] to simulate their experiments in an RCM.

It is recognized that MCH displays the features of low temperature heat release and two-stage ignition behavior; resulting typically from the reactions of peroxy radical. Because the influence of low temperature heat release can become important in practical combustors and engines, a comprehensive detailed reaction mechanism must take the reactions in the low temperature kinetic

regime into account, and should correctly predict the features of autoignition, such as the first- and second-stage ignition delays and the pre-hot ignition heat release.

Experiments in an RCM allow access to conditions of low temperatures where two-stage ignition phenomenon is present. Apart from the recent investigation by Pitz et al. [5] at elevated pressures and low temperatures, there is no other RCM experiment in this operating regime. In this work, in order to provide benchmark experimental data for validating and developing a comprehensive chemical kinetic mechanism of MCH, experiments are conducted for autoignition of MCH in an RCM over a range of compressed charge pressures, compressed gas temperatures, and equivalence ratios. This experimental dataset is then used to assess the performance of an available reaction mechanism taken from [5].

In the following, the experimental and computational specifications are first described, followed by results and discussions of MCH autoignition experiments and model performance.

2. Experimental and computational specifications

Experiments are conducted in an RCM. The details of the present RCM and experimental procedure can be found in [8,9]. Autoignition investigations for three MCH/O₂/N₂/Ar mixtures (denoted as Mix #1–3) are conducted over the compressed gas temperature range of $T_C = 680\text{--}905\text{ K}$ and at two compressed charge pressure conditions of $P_C = 15.1 \pm 0.3$ and 25.5 ± 0.5 bar. Table 1 lists the compositions of the three gas mixtures tested herein.

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Table 1

List of compositions of gas mixtures investigated (in molar proportion).

Mix #	ϕ	MCH	O ₂	N ₂	Ar
1	1.0	1	10.5	12.25	71.75
2	0.5	1	21	0.00	73.5
3	1.5	1	7	16.35	71.15

Moreover, the equivalence ratios corresponding to Mix #1, #2, and #3 are, respectively, $\phi = 1.0, 0.5,$ and $1.5,$ with varying proportions of diluting N₂ and Ar. MCH employed is 99.5% pure (supplied by Fisher Scientific).

In the experiments, the mole percentage of MCH in the reactive mixture is kept constant at 1.047% and the equivalence ratio is varied through variation in the mole percentage of O₂, as shown in Table 1. Additionally, the same specific heat ratio is maintained for all of the mixtures investigated by adjusting the relative proportion of N₂ and Ar in the diluent. The approach of maintaining the same specific heat ratio leads to identical gas temperature and pressure at the end of compression for all mixtures with the same compression ratio and initial conditions of pressure and temperature. For a given mixture composition with initial temperature of room temperature, the compressed gas temperature at the end of compression (top dead center, TDC), T_C , is varied by altering the compression ratio; whereas the desired pressure at TDC, P_C , is obtained by varying the initial pressure of the reacting mixture for a given compression ratio. The temperature at TDC is determined by the adiabatic core hypothesis according to the relation of $\int_{T_0}^{T_C} \frac{\gamma}{\gamma-1} \frac{dT}{T} = \ln[P_C/P_0]$, where P_0 is the initial pressure, T_0 the initial temperature, and γ is the specific heat ratio that is a function of temperature. The value of T_C is taken as reference temperature for reporting the data.

Numerical modeling of RCM experiments is performed using the SENKIN code [10] in conjunction with the CHEMKIN package [11]. The modeling begins from the start of compression stroke, and includes the effect of heat loss during the compression stroke and after the end of compression. In particular, an approach based on ‘effective volume’ is applied to model the effect of heat loss. Description and validation of this heat transfer model are detailed in [8,9,12]. Simulations are conducted using the reaction mechanism of [5].

The experimental pressure traces and the associated empirical effective volume parameters are available in [13].

3. Results and discussion

Fig. 1 shows a typical pressure trace for the ignition of Mix #1 ($\phi = 1.0$) with $T_0 = 296.4$ K and $P_0 = 824$ Torr, along with the definitions of the first-stage ignition delay (τ_1) and the total ignition delay (τ). Specifically, the ignition delays (τ_1, τ) are defined as the time from the end of the compression stroke, where the pressure peaks at $t = 0$, to the corresponding instant of inflection point in the pressure history. For this case, the measured pressure and the deduced temperature at the end of compression ($t = 0$) are $P_C = 15$ bar and $T_C = 705.7$ K, respectively. There is an uncertainty in the reported compressed gas temperature due to the errors associated with the partial pressure measurements for mixture preparation, the dynamic pressure measurements related to the accuracy of piezoelectric transducer, and the initial temperature measurements using a thermocouple. Following the uncertainty propagation approach of [14], the maximum uncertainty in T_C for all experiments is estimated to be less than 3.5 K and is mainly due to the uncertainty in the initial temperature measurement.

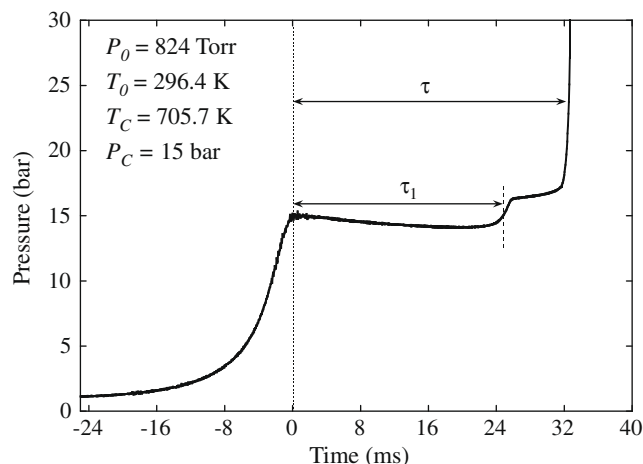


Fig. 1. Pressure trace illustrating the definitions of the first-stage ignition delay (τ_1) and the total ignition delay (τ). Conditions: Mix #1 ($\phi = 1.0$), $P_0 = 824$ Torr, $T_0 = 296.4$ K, $T_C = 705.7$ K, and $P_C = 15$ bar.

Fig. 2 presents the raw experimental pressure traces that are used to obtain the ignition delay results. Each plot in Fig. 2 shows pressure traces for given mixture composition and compressed charge pressure, while varying compressed gas temperature. The pressure traces in Fig. 2 highlight the detailed features observed in the ignition behavior, including the first-stage pressure rise and the hot ignition event. It is seen from Fig. 2 that two-stage ignition response is apparent at low compressed gas temperatures, while single-stage ignition is observed at high T_C . Furthermore, as T_C is increased, the pressure rise due to the first-stage activity decreases and eventually it ceases to exist. This decrease in the first-stage pressure rise with increasing T_C suggests the existence of a cut-off temperature for the first-stage activity. As a result, at low T_C the first-stage activity yields higher pressure rise to attain the cut-off temperature at the end of the first-stage event. It is noted that Griffiths et al. [15] used pressure traces from an RCM to estimate the average gas temperature in the transition from the first stage to the second stage for various alkanes, and reported that the average temperature after the first-stage activity remained approximately constant.

Fig. 2 also shows that for given P_C and T_C , the first-stage pressure rise for an oxygen-rich mixture is higher than oxygen-lean mixture. This behavior is due to the enhancement of peroxidation reactions when O₂ concentration is increased. An increased O₂ concentration also favors low temperature heat release and increases the cut-off temperature for the first-stage activity. It is further seen from Fig. 2 that the limiting value of T_C beyond which the first-stage activity ceases is higher for oxygen-rich mixtures.

Fig. 3 shows the measured τ and τ_1 with varying T_C for different equivalence ratios at $P_C \sim 15.1$ and 25.5 bar. Since ϕ is varied through the change in the mole fraction of O₂ while keeping the mole fraction of MCH constant, the effect of ϕ on ignition delays observed here represents the influence of O₂ concentration. It is seen from Fig. 3 that both τ and τ_1 strongly depend on ϕ and ignition delays increase with increasing ϕ (decreasing O₂ mole fraction). At lower T_C , ignition delays tend to converge and become independent of ϕ . The observed behavior of strong dependence of τ_1 on ϕ (O₂ mole fraction) for MCH is a feature different from the behaviors of other fuels such as dimethylether [16] and *n*-decane [17] that show negligible dependence of τ_1 on ϕ . It is also noted that the onset of negative temperature coefficient (NTC) region is shifted to lower temperatures as ϕ (O₂ mole fraction) is in-

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