



Autoignition of ethanol in a rapid compression machine



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ABSTRACT

Ethanol is a renewable source of energy and significant attention has been directed to the development of a validated chemical kinetic mechanism for this fuel. The experimental data for the autoignition of ethanol in the low temperature range at elevated pressures are meager. In order to provide experimental data sets for mechanism validation at such conditions, the autoignition of homogeneous ethanol/oxidizer mixtures has been investigated in a rapid compression machine. Experiments cover a range of pressures (10–50 bar), temperatures (825–985 K) and equivalence ratios of 0.3–1.0. Ignition delay data are deduced from the experimental pressure traces. Under current experimental conditions of elevated pressures and low temperatures, chemistry pertaining to hydroperoxyl radicals assumes importance. A chemical kinetic mechanism that can accurately predict the autoignition characteristics of ethanol at low temperatures and elevated pressures has been developed and this mechanism is compared with other models available in the literature.

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1. Introduction

Ethanol is a renewable source of energy and is used as a neat fuel as well as an octane enhancer and oxygenate in gasoline. Several investigations have focused on studying the chemical kinetics of ethanol combustion using laminar flames [1–4], shock tubes [5–10], flow reactors [12–14], jet-stirred reactors [15,16] and an RCM [10,11]. Ethanol autoignition has been studied in shock tubes mostly at high temperatures and at pressures of less than 5 bar [5–10]. Few studies have been conducted at elevated pressures and at temperatures lower than 1000 K using shock tubes [8–10] and RCM [10,11]. At low temperatures and elevated pressures, HO₂ radical chemistry can play a dominant role. In an RCM study of methanol autoignition at low temperatures, for instance, it was noted that the reaction of methanol with HO₂ radical is critical to the prediction of ignition delays and the chemistry involving HO₂ radicals is relatively poorly understood with a large uncertainty in rate parameters [17].

Cancino et al. [9] measured ignition delays of ethanol at $\phi = 0.3$ and 1.0 at temperatures in the range 770–1250 K and at pressures of 10–40 bar in a shock tube. Lee et al. [10] determined ignition delay times for stoichiometric ethanol mixtures at 775–1000 K and 80 bar using a shock tube and complemented these with RCM measurements at 35 bar. Limited RCM ignition delay data at 32 bar and

at temperatures lower than 1000 K was also presented in [11]. Autoignition at low temperatures can be influenced by phenomena that are facility specific. In shock tubes for instance, experiments at low temperatures can manifest a pressure rise due to shock attenuation. In addition, significant fuel-specific pre-ignition behavior is sometimes noted where ignition is inhomogeneous to begin with, and is followed by a pronounced deflagrative phase, compression of the unburned mixture and eventual autoignition. In the shock tube study of Fieweger et al. [18], the pressure increase due to the deflagrative phase shortened the time for methanol autoignition by an order of magnitude at 800 K and 40 bar. Medvedev et al. [19] presented an approach to qualitatively determine which shock tube studies may have been affected by pre-ignition phenomena. Given the high sensitivity of induction chemistry to perturbation from shock attenuation and the deflagrative phase, such effects are accounted for in kinetic modeling [20].

By using Schlieren imaging in a shock tube, Lee et al. [10] also noted deflagrative behavior in ethanol autoignition. Pressure measurements as well as emission signals showed strong pre-ignition behavior with pressure increasing by more than 100% in some cases before autoignition. Ignition delays reported without any pressure histories can be highly misleading and could lead to misinterpretation of the experimental data at low temperatures. In contrast to the study of Lee et al. [10], Cancino et al. [9] did not report any pre-ignition pressure rise and adjusted the kinetic mechanism to mimic the plateau in the ignition delay profile at low temperatures. Specifically, a significantly higher value for the rate constant of the

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ethanol + HO₂ reaction was adopted [10]. Consistent with [10], faster ignition in [9] could have been from facility dependent inhomogeneous and strong pre-ignition effects and the adjustment to the HO₂ radical chemistry might be unreasonable.

On the other hand, observed ignition delays in an RCM are typically longer than in shock tubes owing to the conspicuous absence of pressure rise due to shock attenuation that is manifested in shock tubes. The data from a clean RCM is free from the pre-ignition pressure rise that is typical of mild ignition in a shock tube, and the post-compression heat loss can be satisfactorily simulated to isolate chemical kinetic effects. Since the autoignition of ethanol in an RCM has rarely been investigated, the objective of this work is to study this phenomenon and provide useful data for mechanism validation over a range of pressures and equivalence ratios. In the following, the experimental facility is first described followed by the results of the autoignition experiments and a comparison with available kinetic models as well as model refinements.

2. Experimental specifications

Experiments were conducted in a pneumatically driven and hydraulically damped RCM. It has a compression cylinder of 5.08 cm bore and an optimized crevice design to suppress the roll-up vortex. The end combustion chamber of 4.67 cm bore is connected to the compression cylinder through a gradually converging section. This design allows ‘crevice containment’, where the crevice is isolated from the main reaction chamber at the end of compression, which prevents additional mass flow into the crevice when chemical heat release takes place in the main chamber. The specifications of the RCM and the details of the CFD analysis to arrive at the optimized combustion chamber configuration were presented in [21,22]. The compression stroke can be varied between 20.32 and 30.48 cm and the clearance volume is also adjustable allowing for a range of compression ratios up to 16. The dynamic pressure during the experiment is measured using a piezoelectric sensor (Kistler 6052C) and a charge amplifier (Kistler 5010B). The test mixtures are first prepared manometrically inside a 19 L stainless steel tank equipped with a magnetic stirrer and allowed to homogenize before feeding to the combustion chamber.

Autoignition investigations for ethanol/O₂/N₂/Ar mixtures were conducted over the temperature range of 825–985 K, the pressure range of 10–50 bar, and for ϕ from 0.3 to 1.0. The mixture compositions and the ranges of compressed gas pressures and temperatures at the end of compression (top dead center, TDC), P_C and T_C , are given in Table 1. Dilution with N₂ + Ar, required to attain an appropriate value of ϕ within a particular range of compressed gas temperature, was set to be in the same proportion as the non-reactive components in air. For a given mixture composition, the compressed gas temperature within each range (Table 1) was varied by altering the compression ratio, whereas the desired pressure was obtained by independently varying the initial pressure of the reacting mixture. The temperature at TDC, T_C , was determined by the adiabatic core hypothesis according to the relation $\int_{T_0}^{T_C} \frac{\gamma}{\gamma-1} \frac{dT}{T} = \ln[P_C/P_0]$, where P_0 is the initial pressure, T_0 the initial temperature, γ is the specific heat ratio and is a function of temperature.

Table 1
Molar composition of test mixtures.

#	ϕ	Ethanol	O ₂	N ₂	Ar	P_C (bar)	T_C (K)
1	0.3	1	10	8.16	29.44	10, 25, 50	825–985
2	0.5	1	6	1.72	20.84	10, 25	825–985
3	1	1	3	0	11.28	10	860–925

3. Results

3.1. Ignition delay data

An example of a primary pressure trace for autoignition is shown in Fig. 1. The measured pressure and the deduced temperature at the end of compression ($t = 0$) are $P_C = 49.9$ bar and $T_C = 851$ K, respectively. It is also seen from Fig. 1 that the compression stroke is ~ 25 ms, and the ignition delay (τ) is defined as the time from the end of the compression stroke, where the pressure peaks at $t = 0$, to the instant of rapid pressure rise due to ignition. In the case of relatively slower pressure rise during ignition, the inflection point in the pressure trace during ignition is taken as the instant of ignition to determine the ignition delay time. The corresponding non-reactive pressure trace in Fig. 1 also illustrates that the post-compression pressure decay in this RCM is moderate and the pressure falls by less than 7% over a 50 ms interval. The relatively low rate of fall immediately after the piston has stopped, and its subsequent overall extent, is attributed to the prevention of mass flow into the crevice during the post compression period owing to crevice containment. It has been shown elsewhere [21] that a significantly higher rate of pressure decay is manifested during the initial 10 s of ms after compression when crevice containment is not employed. Experimental pressure traces over a range of T_C for $\phi = 0.3$ and $P_C = 25$ bar are shown in Fig. 2 and the pressure rise during ignition is noted to be rapid even at long ignition delays, albeit with a much slower ‘burn out’ in the final stage of combustion.

Figure 3 is a plot of ignition delay times from previous studies of ethanol autoignition, scaled to first order with oxygen concentration, versus the reciprocal of temperature. The present data are also included. The experimental data sets in Fig. 3 have varying fuel loading and equivalence ratio and the purpose is to emphasize the domain of the present experiments in contrast to the previous

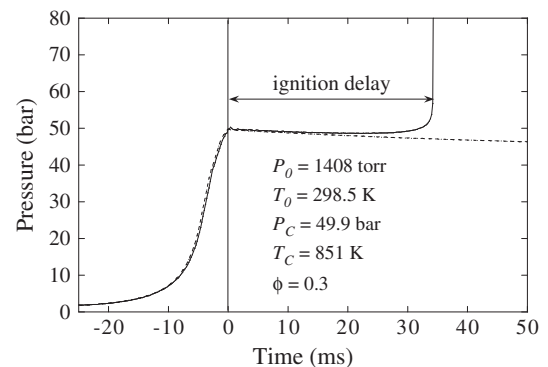


Fig. 1. Typical experimental pressure trace and definition of ignition delay.

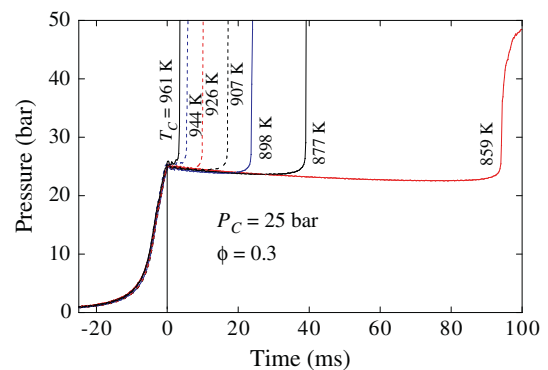


Fig. 2. Experimental pressure traces with variation of T_C , $P_C = 25$ bar, $\phi = 0.3$.

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