



Full Length Article

An ignition delay time and chemical kinetic study of ethane sensitized by nitrogen dioxide



Fuquan Deng^a, Youshun Pan^a, Wuchuan Sun^a, Feiyu Yang^a, Yingjia Zhang^{a,*}, Zuohua Huang^a

^a State Key Laboratory of Multiphase Flows in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, People's Republic of China

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ABSTRACT

Nitrogen dioxide (NO₂) is a dominant component of NO_x pollution in combustion of internal combustion engines and gas turbines. Its sensitization on ignition of ethane which is a main component of natural gas has been investigated in this experimental and kinetic study. Ignition delay times of NO₂/C₂H₆/O₂/Ar mixtures, with blending ratios of NO₂:C₂H₆ of 0.3:1 and 1:1, were measured in a shock tube. Experimental conditions cover a range of pressures (1.2–20 atm), temperatures (950–1700 K) and equivalence ratios (0.5–2.0). Similarly to our previous work of CH₄/NO₂ (Deng et al., 2016) [14], NO₂ addition promotes the reactivity of ethane and reduces the global activation energy particularly at higher pressures ($p > 5.0$ atm) and lower temperatures ($T < 1175$ K), whereas it only presents a limited effect at low pressure (1.0 atm) and higher temperatures ($T > 1175$ K). Furthermore, an opposite effect of NO₂ addition is observed in both the experiments and the simulations at different temperature regimes. Compared to fuel-rich mixture, NO₂ addition exhibits more significantly promoting effect on the ignition of fuel-lean mixture under given NO₂ concentration. Four literature kinetic mechanisms and an updated mechanism proposed in *this study* have been compared to simulate the new ignition delay time data and the literature data. Overall, the proposed model is capable of reproducing the experimental results measured by various facilities over a wide range of conditions. The proposed model is thus used to carry out the sensitivity and flux analyses to clarify the chemistry interaction between NO₂ and ethane. Based on the kinetic analyses, the impact of NO₂ has been expounded at different conditions.

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1. Introduction

Ethane combustion is of interest of gas-engine applications blended with natural gas, coal-bed methane and shale gas. Therefore, proper-understanding of ethane chemistry is of great importance to hierarchically develop a detail kinetic mechanism due to its significance as a critical role of intermediate products in the combustion of hydrocarbon fuels [1,2]. With this in mind, researchers conducted a great amount of fundamental combustion studies of ignition and oxidation of ethane, including ignition delay times [3–6], flame speed [7,8], species concentrations [9,10] and chemical kinetic mechanisms [11–13].

Nitrogen oxides (NO_x) is well known as main gas emissions in engine combustion, and it can be recirculated into the fresh cycle particularly at internal combustion engines with exhaust gas recirculation. The studies reported in our current work [14,15] and literature [14,16,21] have demonstrably indicated that even a very

small amounts of nitrogen oxides can cause a dramatic impact on combustion characteristics of hydrocarbons due to the fact that the presence of NO_x promotes the establishment of radical pool and thus accelerates the oxidation of fuels. Unfortunately, there is only limited work with respect to the chemical interaction of ethane and NO_x. Faravelli et al. [22] studied the combustion characteristics of ethane/NO mixtures at 1.0 atm over a temperature range of 600–1100 K in a plug-flow reactor (PFR) reactor. They proposed a low-temperature NO_x kinetic models and illustrated the impact of NO on the ethane oxidation. Sivaramakrishnan et al. [21] investigated the mutual sensitization of NO and natural gas (CH₄/C₂H₆ = 10:1 in mole fraction) at pressures of 10–50 atm and equivalence ratios of 0.3–1.5 over a temperature range of 1000–1500 K in a high-pressure shock tube and a jet-stirred reactor (JSR). They found that the addition of NO significantly promoted the oxidation of natural gas at the conditions investigated in their study and pointed out that the promoting-effect of NO was caused by the formation of abundant OH radicals via the reaction $\text{H}\ddot{\text{O}}_2 + \text{NO} \rightleftharpoons \text{OH} + \text{NO}_2$. Herzler and Naumann [17] studied the promoting effect of NO₂ (20–250 ppm) on the ignition of CH₄/C₂H₆/O₂/Ar mixtures at 16 bar and equivalence ratios of

* Corresponding author.

E-mail address: yjzhang_xjtu@xjtu.edu.cn (Y. Zhang).

0.25–1.0 over a temperature range of 1000–1700 K in a shock tube. They found that small amount addition of NO_2 can dramatically accelerate the ethane ignition, and the promoting-effect was closely related to the change in equivalence ratios. Clearly, their observation is consensus with the previous work [14,16–21] mentioned above. Gersen et al. [19] performed the study of NO_2 sensitization on two mixtures of $\text{CH}_4/\text{C}_2\text{H}_6/\text{O}_2/\text{N}_2/\text{Ar}$ and $\text{C}_2\text{H}_6/\text{O}_2/\text{N}_2/\text{Ar}$ blend with 100–270 ppm NO_2 at temperatures of 900–1050 K and at pressures of 25–50 bar in a rapid compression machine. For the former mixture, they observed that the addition of NO_2 showed a significantly promoting effect on the reactivity, and this effect increased with decreasing temperatures. However, only a moderately promoting-effect of NO_2 addition was observed for the latter mixture.

Considering the literature review above, it is clearly that the impact of NO_2 on ethane ignition differs from the effect on both pure methane and methane/ethane mixtures. In order to full in the lack of experimental data and understanding of the mutual sensitization of ethane and NO_x , we firstly measure ignition delay times of $\text{C}_2\text{H}_6/\text{NO}_2/\text{O}_2/\text{Ar}$ mixtures over a wide range of conditions. Based on our measurements, Whereafter, we use the new ignition data to evaluate the performances of models by replacement of sub-models of NO_x proposed in literature. Finally, we propose a detailed kinetic model of $\text{C}_2\text{H}_6/\text{NO}_2$ to explore the chemical interaction of NO_2 and C_2H_6 . This work is undoubtedly valuable to design the combustors of gas engines and to develop the NO_x controlling strategies.

2. Experimental

All of the ignition delay times were measured in a stainless steel shock tube, which has been described in detail in our previous study [14,23]. Briefly, the shock tube with a diameter of 11.5 cm is divided into a 4.0 m long driver section and a 4.8 m long driven section by a double-diaphragm machine. Four fast-response pressure transducers (PCB 113B26) connecting with three time-interval counters (FLUKE PM 6690) are equally distributed (30.0 cm interval) at the last 1.3 m of the driven section to measure the incident shock velocities. Before each experiment, the tube was evacuated to below 1 Pa with a mechanical-roots vacuum pump, with a leak rate of less than 1 Pa/min. A piezoelectric pressure transducer with acceleration compensation (PCB 113B03) is located at the end-wall to monitor the reflected shock pressure. Typical pressure rise was evaluated to within 4%/ms due to the physical interaction between the reflected shock waves and boundary layer caused from the incident shock waves. OH^* light emission during the ignition was detected by a photomultiplier (PMT: HAMAMASSU CR131) equipped with a 307 ± 10 nm narrow-band filter.

The $\text{NO}_2/\text{C}_2\text{H}_6/\text{O}_2/\text{Ar}$ mixtures were prepared in a stainless steel tank which was allowed to be static >12 h to ensure sufficient mixing and diffusion. The tank was also evacuated to below 1 Pa with a mechanical-roots vacuum pump system before mixture preparation. The gas purities used in *this study* were C_2H_6 (>99.9%), NO_2

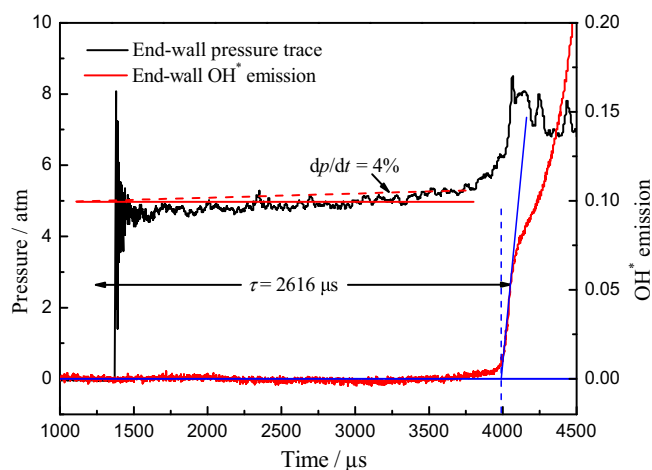


Fig. 1. Typical end-wall profiles of pressure and OH^* emission for $\text{N}_{30/1.0}$ at 5.0 atm and 1044 K.

(>99.9%) diluted with 20% Ar, O_2 (>99.99%) and Ar (99.99%). He (>99.999%) and N_2 (purity 99.999%) were used as the driver gases to achieve a tailored condition. Detailed compositions of the tested mixtures are listed in Table 1.

Fig. 1 illustrates the typical profiles of pressure and OH^* emission. The ignition delay time in this study was defined as the time interval between the incident shock wave arrive at the end-wall, and the onset of ignition detected by both the pressure sensor and the PMT. Clearly, the ignition event monitored by the pressure is in good agreement with that by the light emission. Uncertainty of the ignition delay time was evaluated to within 20% according to our previous study [14].

3. Modeling

The simulations were carried out by CHEMKIN program [24] with SENKIN code [25]. To better reproduce the non-ideal facility effect, the pressure rise (4%/ms) has been considered in all the simulations using SENKIN/VTIM approach proposed by Chaos et al. [26]. Moreover, to eliminate the influence of hydrocarbon chemistry, the state-of-the-art mechanism, Aramco Mech 2.0 [13,27–32] was chosen as the base model of ethane because it has been validated by various data at wide range of conditions. For clarification, we compared the ignition delay times of model predictions and experimental measurements for pure ethane reported in our previous work [1], Fig. 2. It can be seen that the Aramco Mech 2.0 shows an excellent agreement with the experimental data over the studied conditions. Four recently published NO_x models, Sivaramakrishnan et al. [21], Giménez-López et al. [33], Mathieu et al. [18] and Faravelli et al. [22] were integrated into the Aramco Mech 2.0 to evaluate the effects of NO_x sub-models. The four assembled models are thus named Aramco-S, Aramco-G, Aramco-M and Aramco-F, respectively. In addition, an updated model

Table 1
The detail constituents of these mixtures studied in current experiment.

No.	Mix	Mole blending ratio	C_2H_6 (%)	NO_2 (%)	O_2 (%)	Ar (%)	ref
1	$\text{N}_{0/1.0}$	0% NO_2 /100% C_2H_6	1.0	0.0	3.5	95.5	[41]
2	$\text{N}_{30/1.0}$	0% NO_2 /100% C_2H_6	1.0	0.3	3.5	95.2	This study
3	$\text{N}_{100/1.0}$	0% NO_2 /100% C_2H_6	1.0	1.0	3.5	94.5	This study
4	$\text{N}_{0/0.5}$	5% NO_2 /100% C_2H_6	1	0.0	7.0	92.0	[41]
5	$\text{N}_{30/0.5}$	15% NO_2 /100% C_2H_6	1	0.3	7.0	91.7	This study
6	$\text{N}_{0/2.0}$	50% NO_2 /100% C_2H_6	1.0	0.0	1.75	97.25	[41]
7	$\text{N}_{30/2.0}$	5% NO_2 /100% C_2H_6	1.0	0.3	1.75	96.95	This study

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