EXPLOSION PARAMETERS OF AMMONIA/ETHANOL-AIR MIXTURES

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Abstract

The evaluation of burning velocity is essential for the definition of combustion characteristics and the safety assessment of bio-derived fuel-gas mixtures. In this work, the explosion parameters of NH_3/C_2H_5OH-air mixtures have been measured. In particular, the explosion behavior of pure ammonia and ethanol-ammonia in air has been studied for different initial temperatures and equivalence ratios. Experimental tests were carried out in a 5 dm3 closed cylindrical vessel.

Introduction

Bioethanol can be produced from agricultural feed-stocks, forestry wood wastes and agricultural residues [1]. Bioethanol is mainly of interest as a petrol substitute because ethanol-blended fuels undergo cleaner and more complete combustion, thus reducing greenhouse gas and toxic emissions [2]. One of examples for bioethanol production is rice straw, which is the most abundant lingo-cellulosic biomass worldwide [3]. The feedstock is typically pretreated by using ammonia fiber expansion (AFEX) and enzymatically hydrolyzed [4]. Consequently, safe industrial use of this fuel needs explosion data as maximum pressure, maximum rate of pressure rise and burning velocity, which are the most important safety parameters for the safe design of process equipment.

This work aims at studying the explosion behaviour of pure ammonia and ammonia/ethanol in air at different initial temperature and equivalence ratio. To this end, experimental tests were carried out in a closed cylindrical vessel.

Experimental

The experimental set-up adopted in this study is shown in Figure 1. The main reactor is composed by an AISI 316 SS steel, cylindrical vessel (5 dm³), with wall thickness of 5 cm. The mixture composition was obtained by the partial pressure method. Once the set temperature has been reached, the system is vacuumed. For the tests performed with ethanol, a small amount of liquid, which was previously introduced in the sample drum connected to the main chamber under nitrogen atmosphere, is aspired into the main reactor. Once the system reaches the vapour

pressure equilibrium, the system is depressurized to the wished partial pressure, as described in a previous work [5]. Gases were premixed by mechanical stirring (rotating shaft velocity equal to 200 rpm). They were allowed to settle for around 30 s and then ignited by an electric spark (25 kV, 30 mA) positioned at the center of the vessel. Pressure histories were recorded by KULITE ETS-IA-375 (M) series transducers powered by a chemical battery (12 VDC/7 Ah) in order to minimize any disturbance on the output supply, which was recorded by means of a National Instrument USB-6251 data acquisition system (1.25 Msamples/sec). For all tests, the initial pressure was set to 1 bar.
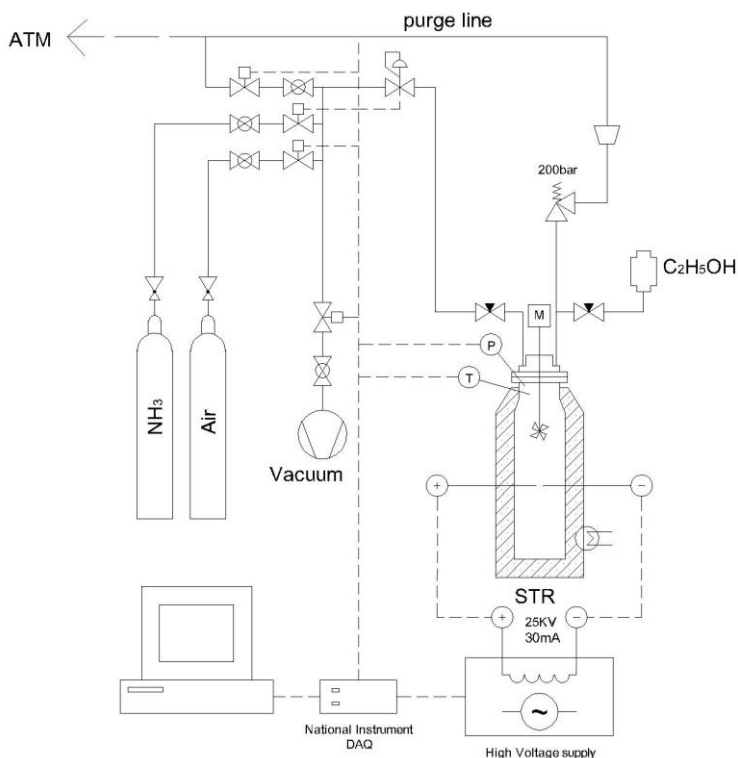

Figure 1. *The experimental set-up adopted for this study.*

The mixture compositions investigated are given in Table 1, together with the corresponding values of adiabatic temperature (T_{ad}) and pressure (P_{ad}) at constant volume, as computed using the GASEQ Chemical Equilibrium Program [6]. The laminar burning velocity was obtained from the time pressure record of the explosion occurring in the closed vessel. In particular, we used the equations by Dahoe et al. [7,8] that link the flame radius, r_f, and the laminar burning velocity, S_l, to the pressure time history.

Table 1. Mixture compositions analyzed in this work: φ is the equivalence ratio; Y is the molar fraction; T_{ad} and P_{ad} are the adiabatic temperature and pressure, respectively, as calculated using GASEQ [6]; P_{max} and S_l are the maximum pressure and the laminar burning velocity, respectively, as found experimentally.

N	φ, -	T, K	Y_{NH3}, -	Y_{C2H5OH}, -	Y_{air}, -	T_{ad}, K	P_{ad}, bar
1	0.8	300	18.3	0	81.7	2241.1	7.8
2	0.9	300	20.1	0	79.9	2369.6	8.3
3	1.0	300	21.9	0	78.1	2460.4	8.7
4	1.1	300	23.5	0	76.5	2443.8	8.8
5	1.0	373	21.9	0	78.1	2497.7	6.6
6	1.0	300	3.6	5.5	90.9	2540.5	9.1
7	1.0	300	7.6	4.3	88.1	2524	9.0
8	1.0	373	3.6	5.5	90.9	2566.4	6.9
9	1.0	373	7.6	4.3	88.1	2552.1	6.9

The flame radius was calculated by using the following correlation:

$$r_f = \left(\frac{3V}{4\pi}\right)^{1/3}\left[1-\left(\frac{P^\circ}{P}\right)^{1/\gamma}\left(\frac{P_{max}-P}{P_{max}-P^\circ}\right)\right]^{1/3} \tag{1}$$

where P_{max} is the maximum measured pressure, P° is the initial pressure, and V is the vessel volume. The (un-stretched) laminar burning velocity, S_l, was then calculated according to:

$$S_l = \lim_{r_f \to 0}\left[\frac{d}{dt}r(t)\right]_{\Delta r_f} \tag{2}$$

where r(t) is the best fit function in the range $\Delta r_f = (r_f - r_{f,o})$ that refers to the range of the flame radius for which either ignition or wall and vessel shape effects on the flame propagation can be neglected. Further details on the methodology can be found elsewhere [9].

Results

The experimental pressure time histories of Figure 2 show the effect of equivalence ratio and temperature. The maximum pressure reached during the experiments is always lower than the corresponding adiabatic value due to the presence of heat losses toward the external environment. The increase of air content (Figure 2, top) and temperature (Figure 2, bottom) significantly increases the maximum pressure (P_{max}) and the rate of pressure rise. From the pressure time histories, we also computed the laminar burning velocity (S_l). The calculated values of maximum pressure (P_{max}), maximum pressure rise [$(dP/dt)_{max}$], and burning velocity (S_l) are given in Table 2.
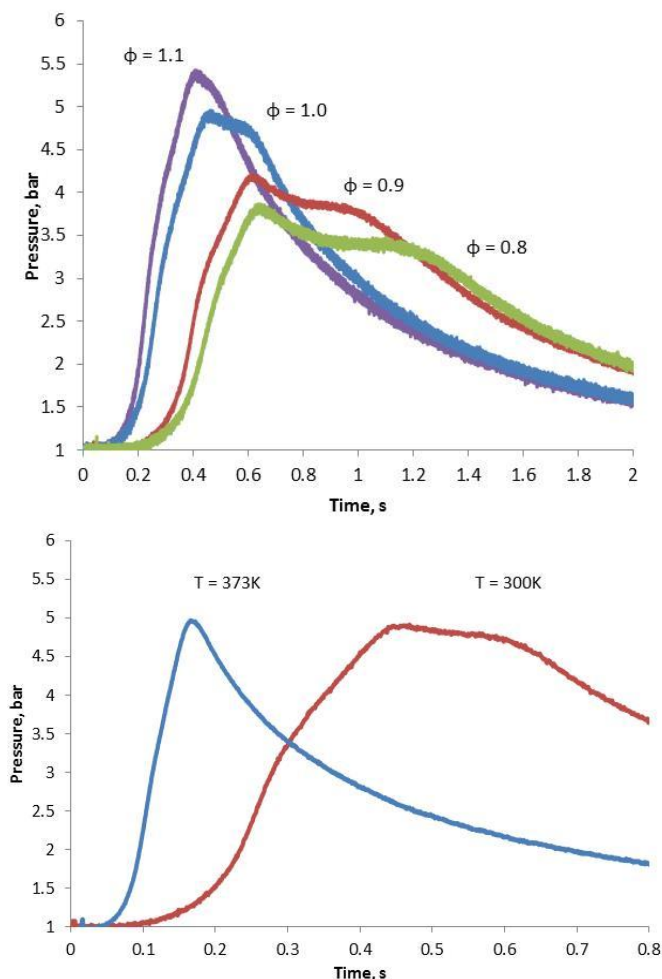
Figure 2. *Experimental pressure time histories as measured at different equivalence ratios (top) and temperatures (bottom) for ammonia/air explosion.*

Figure 3 shows the experimental pressure time histories obtained for C_2H_5OH/NH_3/air mixtures at 300 K (Figure 3, top) and 373 K (Figure 3, bottom). An increase of initial temperature is reflected in the increase of reactivity (S_l, and maximum rate of pressure rise, i.e., $(dP/dt)_{max}$).
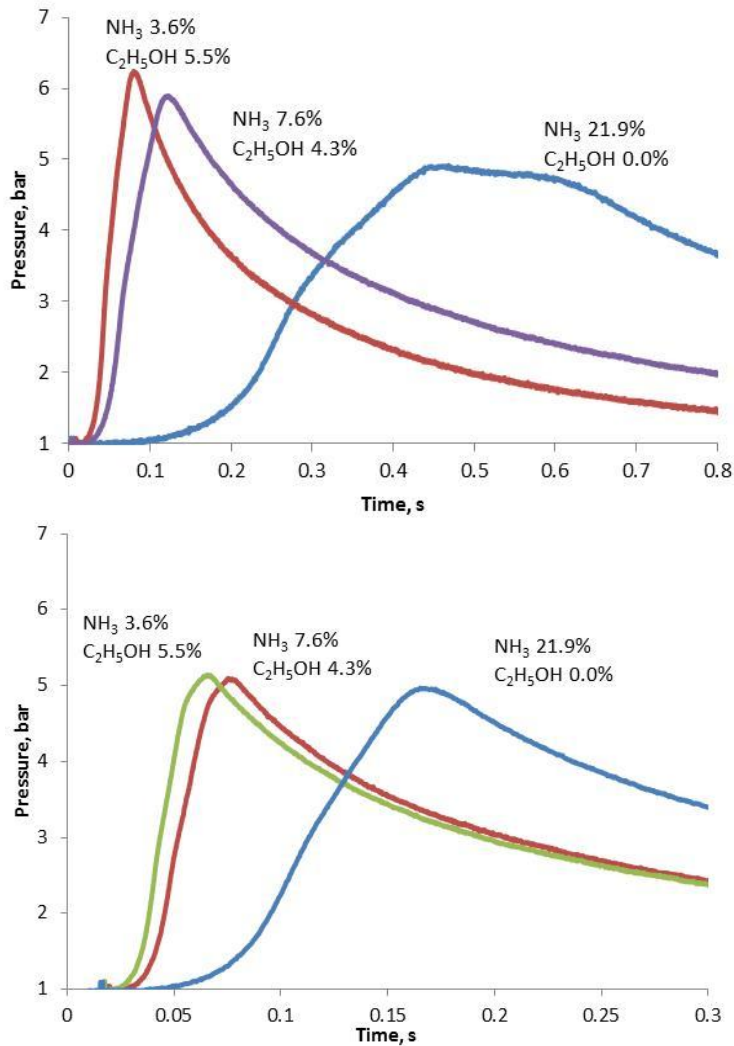
Figure 3. *Pressure time histories as measured for ammonia/ethanol/air at 300 K (top) and 373 K (bottom)*

The values of P_{max}, $(dP/dt)_{max}$ and S_l as extracted from the time histories of Figure 3 are given in Table 2.

Conclusions

The effects of temperature, equivalence ratio and ethanol enrichment factor on the laminar burning velocity of NH_3/air mixtures have been experimentally quantified. The burning velocity is generally very low even at stoichiometric conditions, but it is strongly affected by temperature.

Table 2. P_{max}, $(dP/dt)_{max}$ and S_l for all the experimental conditions investigated in this work.

N	φ	T, K	P_{max}, bar	$(dP/dt)_{max}$, bar s^{-1}	S_l, m s^{-1}
1	0.8	300	3.8	17.7	0.07
2	0.9	300	4.2	20.9	0.07
3	1.0	300	4.9	27.0	0.09
4	1.1	300	5.4	34.3	0.09
5	1.0	373	5.0	30.7	0.15
6	1.0	300	5.9	54.1	0.24
7	1.0	300	6.2	63.5	0.17
8	1.0	373	5.1	70.7	0.32
9	1.0	373	5.1	59.4	0.29

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