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Influence of pressure, temperature and vessel volume on explosion characteristics of ethanol/air mixtures in closed spherical vessels

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HIGHLIGHTS

- Experimentally determined explosion parameters of ethanol/air mixture.
- Influence of initial conditions on the explosion characteristics.
- Linear correlations between the explosion pressures and the initial pressure.
- Linear correlations between the rates of pressure rise and the initial pressure.

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ABSTRACT

Ethanol is a biofuel that can be used as an alternative fuel or as a blending component for combustion engines. This requires more information and systematic investigation of the explosion parameters of ethanol in air under various conditions. The most frequently used pressure-related parameters for risk assessment – the maximum explosion pressures, the maximum rates of pressure rise, the severity factors and the maximum explosion delay time – are determined in two spherical vessels (volume: 0.005 m^3 and 0.020 m^3) for various ethanol/air mixtures (3.5–20.0 vol%) at various initial pressures (10.1–101 kPa) and temperatures (298–373 K).

1. Introduction

Decreasing reserves of fossil fuels and current regulations for emissions from internal combustion engines that affect the environment and human health have stimulated a pronounced interest in nonconventional fuels and fuel additives. Alcohols derived from agricultural residues, feed-stocks and forestry wood wastes by means of biochemical processes have the potential to provide a path towards renewable, carbon-neutral fuels.

Ethanol is considered to be one of the most important alternatives to gasoline, as its use can lead to reductions in consumption of fossil fuels and in environmental pollution. In a number of recent studies on practical engines, reductions in NOx and particle emissions were observed when ethanol was added [1–3]. Moreover, the production of ethanol from biomass can negate the effect of the carbon dioxide emitted during the combustion process.

The combustion reactions of ethanol have been investigated experimentally and in mechanistic studies [4–8]. Ethanol combustion has been studied in a low-pressure flame [5], in a laminar premixed flame [9,10], in a diffusion flame [11], in a jet-stirred reactor (JSR) [12], in a flow reactor [13,14], and in a shock tube [15–17]. The laminar burning velocity of an ethanol/air mixture has been investigated using the following different experimental techniques: a combustion bomb [18–23], a counter-flow flame [24], the heat flux method [25] and a cylindrical vessel [26–29]. The laminar burning velocity of gasoline with the addition of ethanol has been investigated as well [28]. Measurements of the laminar burning velocities of n-heptane, iso-octane, ethanol and their binary and tertiary mixtures have been reported [29]. The explosion parameters and the effect of hydrogen addition on the explosion of ethanol/air mixtures (among other subjects) have been reported by Cammarota et al. [30,31].

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Nomenclature

d	diameter
p	pressure (kPa)
T	temperature (K)
K	deflagration index
t	time (s)
V	volume (L)
a, b	slope and intercept of the correlation p_{max} against p_0
m, n	slope and intercept of the correlation $(dp/dt)_{max}$ against p_0
r_n^2	the regression coefficient
l	length

Greek letters

θ	time-to-peak pressure
Δ	variation
φ	equivalence ratio of fuel/oxidant mixtures
$\pi\alpha$, β	slope and intercept of the correlation π_{max} against $1/T_0$

Subscripts

0	initial value
ex	explosion
G	referring to gas explosions
max	maximum value
s	sphere

A study of auto ignition temperatures, explosion limits, explosion points and the maximum experimental safe gaps of ethanol/gasoline mixtures was conducted by Brandes et al. [32]. A study of the explosion characteristics of short-chain alcohols was carried out by Mitu and Brandes in [33]. A comparative assessment of the explosion characteristics of alcohol/air mixtures was recently presented by Li et al. [34] using a constant-volume vessel. Brooks and Crowl [35] carried out experiments on the flammability of some alcohols using a spherical vessel with a fuse wire igniter.

However, additional information is required with respect to the explosion characteristics of ethanol in air under various initial conditions.

The maximum explosion pressure, the maximum rate of pressure rise and the gas deflagration index K_G are the most important safety parameters of combustion dynamics in the deflagration regime used to describe the effect of an explosion. These parameters are also needed to evaluate the flammable hazards of chemical processes, the design of explosion-proof vessels and the design of vents in order to mitigate the effects of gas explosions [36]. These parameters depend on the following initial conditions: the composition, temperature and pressure of the flammable mixtures and the volume and form of the vessel [37–41]. In any technological process where flammable mixtures occur, it must be taken into account that the design of the vent areas, the type of safety valve and the vent set pressure may depend on the initial conditions (temperature, pressure) and on the geometry. Measured explosion parameters of ethanol/air mixtures under a wide range of initial conditions increase the information available from databases of the explosion parameters of fuels.

The aim of the investigations reported here was to characterize the explosion of ethanol/air mixtures (explosion pressure, rate of pressure rise, deflagration index, explosion delay time) in closed vessels under different initial conditions of concentration, pressure, temperature and vessel volume.

2. Experiments

The measurements carried out on ethanol/air mixtures were performed in two closed vessels with different volumes (0.005 m^3 and 0.020 m^3), using central ignition according to EN 15967 [42]. The set-up, designed in accordance with EN 15967, consisted of a spherical stainless-steel vessel, an evaporator tube to evaporate the liquids, a mixing vessel to homogenize the vapor/air mixture, metering devices for ethanol and air, a heating system and a pressure-measuring system. A series of induction sparks between two stainless-steel electrodes (1 mm diameter, angle of the pointed tips: 60° ± 3°) was used as ignition source. The distance between the tips was 5 mm ± 0.1 mm. The power of such an arrangement depends on the gas mixture and initial pressure. In air at atmospheric conditions such an arrangement gives a power of approximately 10 W. The ignition source was mounted such that the electrodes end in the center of the sphere [42]. Other details on the explosion vessel and on the preparation of flammable mixtures are given in a previous publication [43].

Ethanol (99.9%) was used without further purification. The equivalence ratio φ of the mixtures studied was between 0.52 and 3.57 ([C_2H_5-OH] = 3.5–20.0 mol%). (The equivalence ratio φ is defined as: $\varphi = \frac{[fuel]/[oxygen]}{([fuel]/[oxygen])_{st}}$, where the index "st" refers to the stoichiometric concentration of the fuel/air mixture.)

The initial pressures (p_0) studied were between 10.1 kPa and 101 kPa, at variable initial temperatures (T_0) between 298 K (p_v: 7.8 kPa) and 373 K (boiling point: 78 °C; p_v > 100 kPa).

Normally, three tests were carried out for each composition and condition. For the concentration at which p_{max} or $(dp/dt)_{max}$ was found, five tests were carried out.

3. Data evaluation

For all of the mixture compositions investigated (3 tests/5 tests) the mean is given as a result or used in further evaluations. Except for the mixture compositions with the lowest amount of ethanol and those with $\varphi > 3$, the scatter of each value is within the requirements of EN 15967 [42]. As an example see Table 1.

The computation of *(dp/dt)* from the *p(t)* diagrams was carried out after smoothing the *p(t)* data by means of the Savitzky-Golay method (low-degree polynomial fitting based on linear least squares across a moving window within the data). This method has the advantage of producing a smoothed first derivative without filtering the data.

The experimental values of the deflagration index $K_{G,ex}$ of each mixture composition were determined using Eq. (1) [36]:

Table 1
Values of the explosion pressures (p_{ex}) of 7.04 mol% C_2H_5-OH in air, 0.005 m^3 vessel.

T_0/K	p_{ex}/kPa		
	p_0 = 101 kPa	p_0 = 75 kPa	p_0 = 50 kPa
	814.9	615.2	402.3
323	826.2	611.3	405.3
	817.9	607.4	405.8
	715.3	538.0	358.9
373	710.5	539.0	359.4
	710.9	540.5	359.2