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Influence of Initial Temperature on Explosion Severity Parameters of Methanol/Air Hybrid Mixture Measured in 1-m^3 Vessel

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The maximum explosion pressure (P_{max}), the deflagration index (K_G) and the explosion duration (t_{ex}) have been determined in spherical explosion vessel (1 m^3) for various methanol/air mixtures concentrations (6.0-25.0 vol. %) at ambient initial pressure (101 kPa) and three initial temperatures (25 °C, 50 °C,100 °C). The outcome of this preliminary study is to quantify the dependency of explosion parameters on two variables - methanol concentration (C) and initial temperature (T_0), respectively.

1. Introduction

Any change in the initial absolute pressure of the fuel–oxidant mixture at a given initial temperature produces a proportionate change in the maximum pressure developed by a deflagration of the mixture in a closed vessel (NFPA-68-2007). Effect of test volume on K_G measured in spherical vessels is pronounced for many initially quiescent gases and the normalized K_G index is found not to be constant but to increase with vessel volume. The increase in K_G is related to various flame acceleration effects, as described in (NFPA-68-2007). Therefore, K_G, values that are measured in vessels of different sizes cannot be compared directly, even if all other factors affecting K_G are held constant. Any K_G measurement should be made in a spherical vessel at least 5 L (0.005 m^3) in volume, and the values obtained should be corrected based on the 1 m^3 volume. The classification work carried out in the 1 m^3 vessel provides the only direct link between small-scale closed vessel tests and the large-scale vented tests (NFPA-68-2007).

Methanol is an alternative, renewable, environmentally and economically attractive fuel; it is considered to be one of the most favourable fuels for conventional fossil-based fuels. Methanol has been recently used as an alternative to conventional fuels for internal combustion (IC) engines in order to satisfy some environmental and economic concerns. Because of a number of relatively large research projects that have been ongoing recently, much progress has been made that is worth reporting (Zhen & Wang, 2015).

The evaluation of methanol as an alternative fuel requires, among other things, information and the systematic investigation of explosion parameters of methanol in air in various conditions (Mitu & Brandes, 2015). Where the hazard consists of a flammable gas mixture, the vent size shall be based on the K_G or fundamental burning velocity of the mixture. For gases, p_{max} shall be determined in approximately spherical calibrated test vessels of at least 5 L (0.005 m^3) capacity with initially quiescent mixture with low energy ignition source (less than 100 J) (NFPA-68-2007).

Li et al., 2015a) studied the explosion characteristics of five alcohole-air (ethanol, 1-butanol, 1-pentanol, 2-pentanol and 3-pentanol) mixtures in an isochoric chamber over wide ranges of initial temperature and pressure. The effect of temperature (120-160 °C) and pressure (0.1-0.75 MPa) on the different explosion behaviors among these alcohols with various structures were investigated. (Li et al., 2015b) studied the explosion characteristics of four pentanol isomer–air mixtures (n-pentanol, 3-methyl-1-butanol, 2-methyl-1-butanol, 2-methyl-2-butanol), at various initial temperatures (120-200 °C) and initial pressures (0.1-0.25 MPa). (Mitu & Brandes, 2015) measured the explosive combustion of methanol–air mixtures at various initial conditions – temperatures (50-100 °C), pressures (0.05-0.10 Mpa) and fuel/air ratios (0.54-2.26) within the explosion limits in a 0.005 m^3 closed vessel with central ignition. (Mitu & Brandes, 2017) measured the

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maximum explosion pressures, the maximum rates of pressure rise, the severity factors and the maximum explosion delay time 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 (25–100 °C). (Saeed, 2017) implemented a new multizones model to experimentally determine fundamental explosion characteristics of methanol-air mixtures using a closed vessel (160 mm internal diameter). He studied the methanol-air mixtures at different initial conditions of temperature (up to 202 °C), pressures (up to 0.35 MPa) and equivalence ratios (0.7-1.5). (Hu et al., 2017) experimentally investigated and analysed the effects of n-butanol addition on the explosive characteristics of iso-octane-air mixtures with various concentrations and initial pressures and temperatures on the basis of combustion pressure history.

Most explosion characteristics published so far are valid limited experimental conditions, mostly ambient. There are just few of data covered the high initial temperatures which are limited to low volume experimental devices. There are discrepancies in the explosion severity characteristics measured by different researchers for the same methanol / air mixture. There have been no explosion characteristic exists for methanol / air mixtures which cover industrial conditions up to 100 °C in 1 m^3 standard.

2. Experiment

2.1 Experimental set-up

The chamber is a vessel of a spherical shape with an inside diameter of 1240 mm and a capacity of 1 m^3 made by OZM Research, s.r.o. Schematic representation of the whole system is shown at Figure 1.

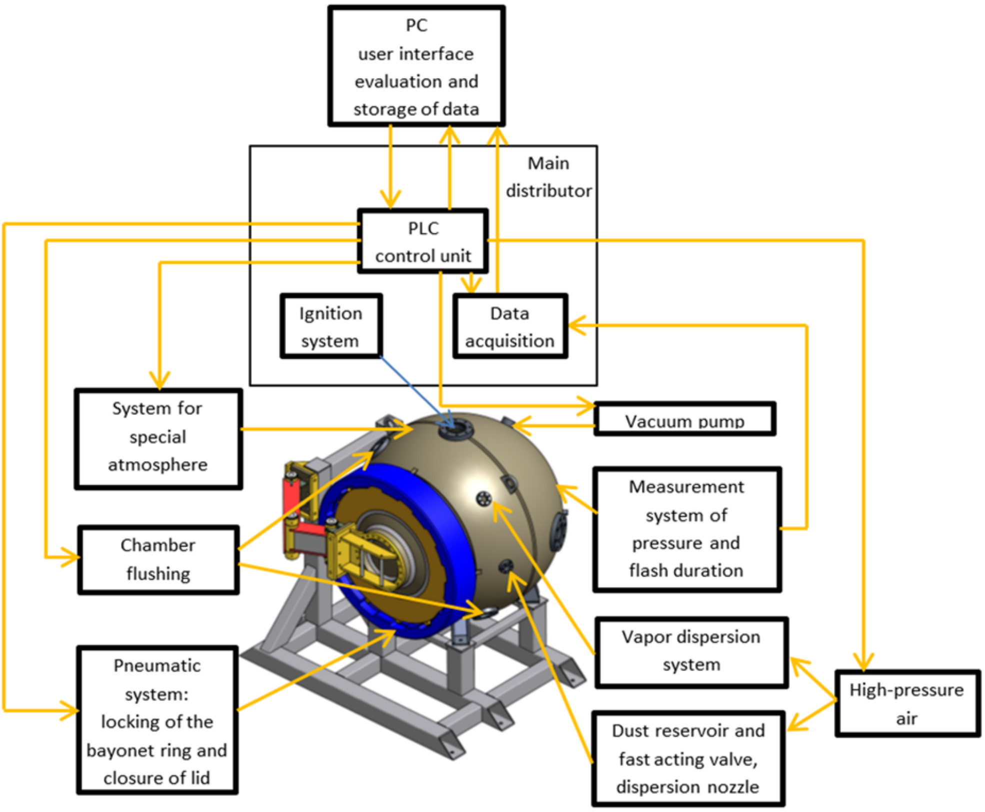

Figure 1: Schematic arrangement of the 1 m^3 chamber with heating system.

The material and components comply with the use of equipment for experiments at atmospheric initial pressure and different initial temperatures (15-200 °C). The explosion chamber is equipped with measurement of time depended dynamic pressure using two pressure sensors by Kistler type 701A calibrated for the range up to 2.5 MPa. Natural frequency of the sensor is 70 kHz. Data are recorded be four-channel data card with a sampling rate 50 kS/s/channel. PLC Siemens Simatic 1215 connected to PC used as a user interface automatically control whole procedure including fast acting valve timing. The chamber is equipped by thermocouple for temperature monitoring, especially for measurement of temperature in time of ignition.

Correct vapour mixture composition is assured by partial pressure method. Pressure transducer measures internal pressure. Procedure for vapour gas explosion starts with evacuation to pressure less than 89 kPa to leave a space for the vapour. PLC starts the experiment where 600 ms is counted as ignition delay time, and then the gas is mixed by blowing dispersion air into the methanol/air mixture inside the chamber. Electric discharge according to EN 15967 was used as ignition source (less than 100 J). Procedure for vapour explosion starts with evacuation to pressure less than 0.89 bar to leave a space for the vapour. For example, the use of methanol concentrations of 5 vol. % and 10 vol. % require the partial pressures of methanol to be added are 0.05 bar and 0.10 bar respectively. Then the evacuation pressures should be 0.84 bar and 0.79 bar respectively. PLC starts the experiment where 600 ms is counted as ignition delay time, and then the gas is mixed by blowing dispersion air into the methanol-air mixture inside the chamber. After that the mixture is ignited by the electric discharge.

2.2 Calculation procedure

For all eleven different concentrations of the methanol-air mixture, a calculation method of minimizing free Gibbs energy was used. The calculation procedure is described in (Skrinsky and Skrinska, 2014a). For each concentration, the experimental explosion pressures (P_{ex}) were compared with the numerically calculated adiabatic explosion pressures (P_{ad}) under the assumption of chemical equilibrium reached in the flame front. As input parameters, the kinetic mechanisms and thermodynamic data sets (C_p, S_0, H_0, G_0) were used primarily from THERMO.dat databases of (Explosion Pressure, 2004) and Thermdat.tdd from (GASEQ, 2005) in CHEMKIN standard polynomial format.

3. Results and discussions

The dependency of explosion parameters on two variables - methanol concentration (C) and initial temperature (T_0) are presented for 1 m^3 constant volume chamber with heating system.

3.1 Influence of the concentration

Figure 2 plots the p_{ex}/time curves at 15-21 vol % methanol/air mixtures at p_0 = 101 kPa in T_0 = 50 °C in 1 m^3 spherical vessels.

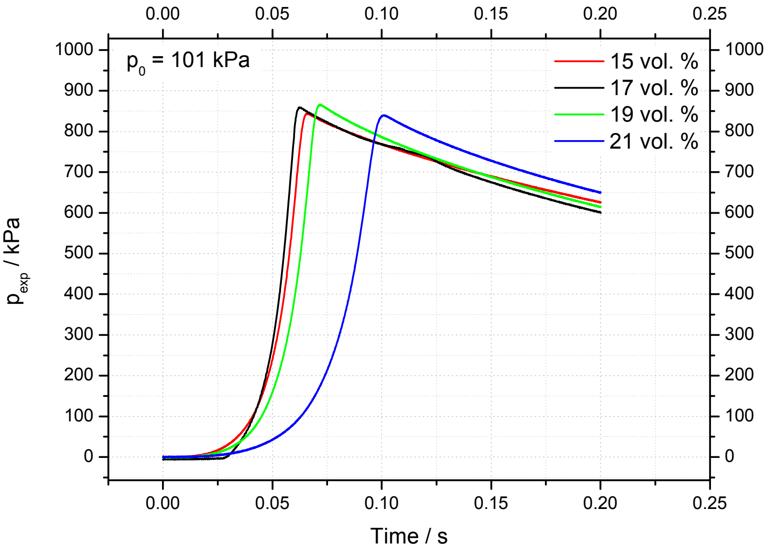

Figure 2: P_{ex}/time curves during the explosion of a 15-21 vol % methanol/air mixtures at P_0 = 101 kPa in T_0 = 50 °C in 1 m^3 spherical vessel

Figure 2 shows that under P_{max} (860 kPa) pressure reached its maximum most rapidly at concentrations of 17 vol. %, while the t_{ex} gradually increase and the p_{ex} decrease with the mixture getting richer. Figure 3 plots K_G/time curves during the explosion of a 15-21 vol % methanol/air mixtures at p_0 = 101 kPa in T_0 = 50 °C in 1 m_3 spherical vessel.

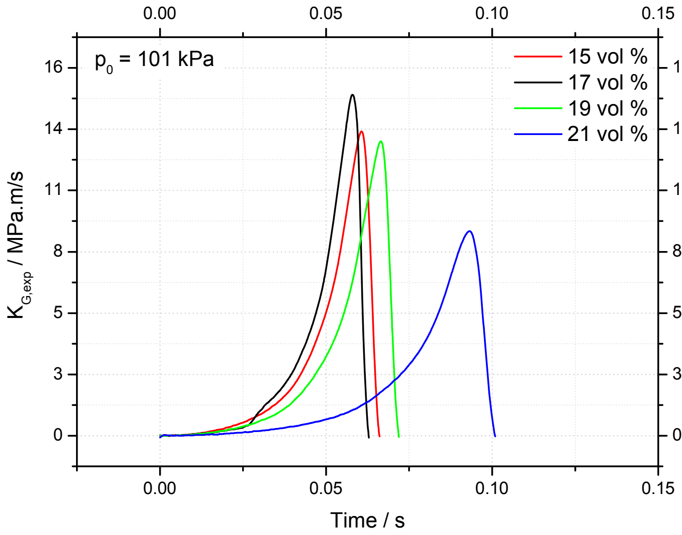

Figure 3: K_{Gexp}/time curves during the explosion of a 15-21 vol % methanol/air mixtures at P_0 = 101 kPa in T_0 = 50 °C in 1 m^3 spherical vessels

The explosion pressures hit top and the explosion durations hit bottom at concentration 17 vol. %. Accordingly, the maximum K_G hits its top here. When it comes to lean burn limit or rich limit of mixture, things go to the reverse side, as shown in Figure 2.

3.2 Influence of the initial temperature

The p_{max} and $(dp/dt)_{max}$ (time derivatives of the explosion pressure) and t_{ex} (the time at which the maximum explosion pressure is reached) were derived from the recorded pressure/time curves. Figure 4 shows p_{ex}/p_0 at three methanol/air T_0 for ambient initial pressure (p_0 = 101 kPa).

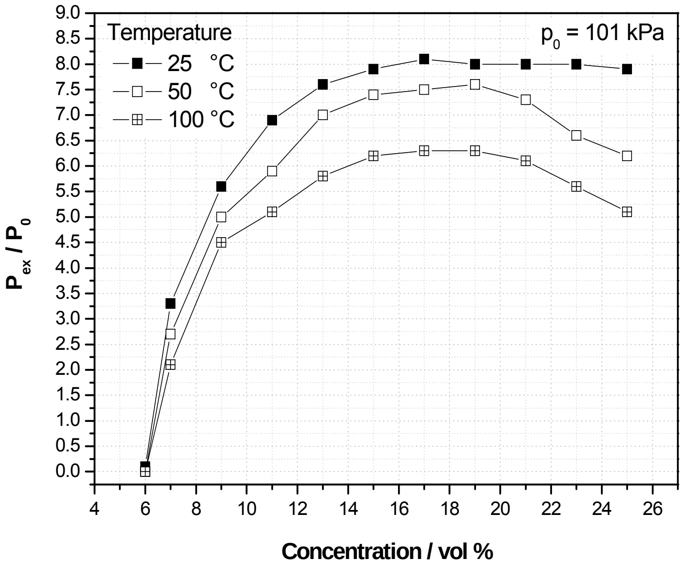

Figure 4: Pex/P0 at various methanol/air initial temperatures (T0) for ambient initial pressure (P0 = 101 kPa).

For the lean and stoichiometric (more than 17 vol. %) mixture compositions investigated, there is Antoine´s limit. With any change in concentration, it is not possible to achieve a higher saturation vapor pressure and the p_{exp} value remains constant and does not decrease towards the UEL. At T_0 = 25 °C , evaporate 0.055 MPa and at T_0 = 100 °C evaporate 0.353 MPa of the total amount of methanol to be dispersed. This is the same for all tested concentrations of alcohols. This phenomenon affects the dependence of p_{max} vapor of liquids on temperature overall. p_{exp} first increases to the point where the vapor maximum is reached, and when the saturation vapor pressure exceeds the increasing temperature decreases for all the studied mixtures.

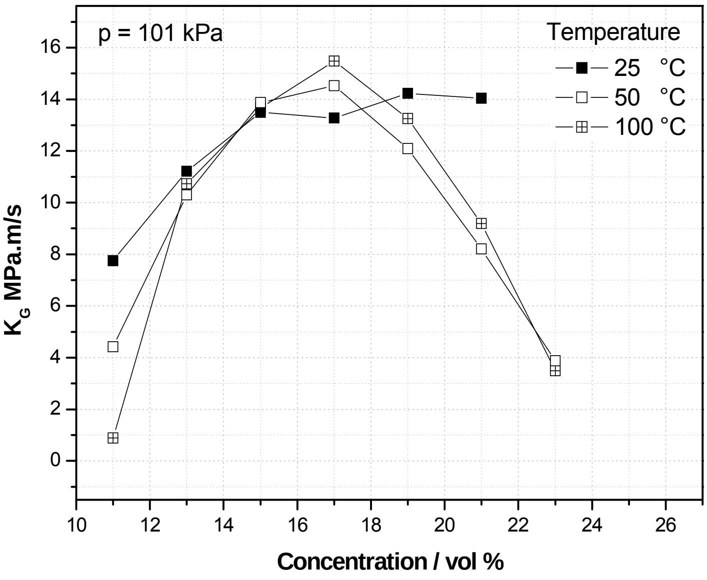

Figure 5: K_G at various methanol/air concentrations (C) and initial temperatures (T_0) for ambient initial pressure (P_0 = 101 kPa).

Figure 5 shows the variation of K_G with concentrations and initial temperatures (T) for methanol as measured in 1 m^3 spherical test vessel. The increase in K_G is related to various flame acceleration effects, as described in (NFPA 68, 2002). At all initial temperatures, the K_G has been observed at concentration where p_{max} has been found. Deflagration indexes have maximum at 17 vol. %, and their values decrease going to lean and rich mixtures. K_G gives the similar peak value at varied initial temperatures, indicating that K_G are insensitive to the variation of temperature.

The resulting values are summarized in Table 1, where the measurement uncertainties are determined by the test method.

Table 1: Values of explosion characteristics for the most reactive methanol/air mixtures at P_0 = 101 kPa.

Parameter	**Unit**	**Value**		
		25 °C	50 °C	100 °C
P_{max}	(kPa)	910±30	860±30	780±30
K_G	(MPa.m/s)	13.3±0.5	14.5±0.5	15.5±0.5
t_{ex}	(ms)	73	66	60

4. Conclusions

Energy Research Centre, VŠB-TU Ostrava is aimed at fundamentally improving the understanding of gas / vapor oxidation processes, the risk assessment of such processes, their environmental efficiency and safety (Skrinsky et al., 2016). The explosion severity parameters have been determined as maximum explosion pressure, the deflagration index, and the time to reach the maximum explosion pressure of methanol-air mixture. All parameters have been measured in an enclosed spherical vessel of 1 m^3 with a central initiation and calculated in various initial conditions of temperature and fuel/air concentrations. The highest values have been evaluated at concentration corresponding to 17 vol % that is above the stoichiometric concentration (12 vol. %). The results support comparative studies on the explosion characteristics of methanol-air mixtures at ambient and elevated temperatures. Present values of explosion characteristics can be practically used in designing explosion protection techniques, such as explosion-proof design, explosion relief, and explosion suppression. They can also be used to eliminate the risk of explosion by preventing the formation of an explosive vapour mixture.

The main conclusions are summarized as follows:

1. Explosion pressure, rate of explosion pressure rise and deflagration index of the methanol mixture reach maximum values near the stoichiometric concentration at 17 vol. %, within the studied range, i.e. 6-25 vol. % at initial temperatures 25 °C, 50 °C,100 °C and initial pressure of P_0 = 101 kPa.
2. The explosion pressure, the rate of explosion pressure rise and the deflagration index of the methanol / air mixture decrease with the increasing initial temperature for the given measurement conditions.
3. t_{ex} values slightly decrease with increasing temperature from 73 ms to 60 ms for 25 °C and 100 °C.

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