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SIMULATION OF PROPANE EXPLOSION IN CLOSED VESSEL

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Abstract: Dust and gas explosions occur in a wide range of industrial segments. They can cause significant harms, when they happen in closed areas, like industrial enclosures, vessels, pipelines, elevators, etc. Evaluation of the possible size of harms based on explosibility of substances, maximum explosion overpressures and maximum pressure rises. Exact measurements in industrial enclosures are greatly dangerous, because load bearing capacity of equipment is finite, and in case of any damage needed to grant proper safety for living beings and environment. Totally explosion-proof enclosures are used mainly in laboratories, which are proper for specifying explosion characteristics of different materials. This article investigates propane explosions in a closed spherical vessel based on experimental and simulation data. The vessel was a 20-liter spherical explosion chamber by Kühner, and 5 vol. % propane-air mixtures were investigated in it. A numerical model was elaborated to simulate concentration changing of materials and pressure rise during explosion process in closed vessel, based on reaction-kinetics. Numerically simulated pressure rise and measured ones were compared.

Keywords: Propane Explosion, Numerical Simulation, Pressure Rise, Reaction Kinetics. One-equation Model

1. INTRODUCTION

Explosive gases and dusts are handled in various industrial segments, from food industry to chemical corporations. Dust and gas explosion phenomena have been studied for decades, although results are still far from their required level. Lots of ordinary summarizing publication can be found in the literature which clearly negotiate cases and causes of explosions, rule standards and opportunities of safety – Barton's. [1], Eckhoff's [2] and Amyotte et al. [3] work deserves attention in the topic.

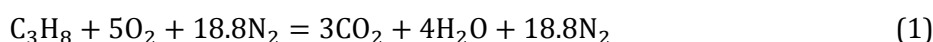
The first line of safety is prevention, which means avoidance of explosions. Some possibilities are given and many devices are commercially available, however combination of circumstances should result further disaster. Practically, there is impossible to completely avoid explosions.

Production processes, transport and storage are take place mostly in closed enclosures. In case of unexpected explosion, pressure significantly rises in the closed volumes in a few milliseconds. For explosive materials, a few typical values describe their capability and characteristic of explosion. Most important ones are maximum explosion overpressure and maximum rate of explosion pressure rise. Maximum explosion overpressure (p_{max}) developed in a closed vessel during the explosion of an explosive atmosphere and determined under specified test conditions. Maximum rate of explosion pressure rise per unit time during explosions of explosive atmosphere in a closed vessel determined under specified test conditions. [4]

However, real industrial situations are far different from test conditions, and which are uneasy to reproduce amongst laboratory circumstances. The most reliable calculation methods for this problem are those numerical simulations which are validated by experimental data.

Propane is an important fuel, and its combustion properties are nearly independent from ignition energy, therefore further investigations of this paper deal with a 5 vol. % mixture with air of this material.

While air approximated with mixture of 21 vol. % of Oxygen, and 79 vol. % of Nitrogen, the base chemical reaction takes place as Equation 1:



However, during high temperature combustion of propane, it characterized by the rapid decomposition into smaller intermediates. Chemical kinetic modelling has become an important tool for understanding





the combustion phenomena. [5] Those models give the supreme approach, which are based on full kinetic mechanism of the chemical reaction [6], but even reduced kinetic mechanisms are composed of more than 30 equations. [7] They can be solved with asymptotic analysis, which estimates proper differential equations for concentration-changing, using reaction rate constants estimated by modified Arrhenius-equation. [8]

Much more simple reaction models are one-equation models, which are presuppose premixed combustion in every point of the measured volume. These models give a differential equation of fuel concentration to time. One early model is Westbrook's mechanism [9], however it is not consider pressure during estimation, like a few state-of-the-art publications, too. [10] Frolov et al. in their some writings discuss the topic taking into consideration pressure changes during combustion process, and shows progressive improvement in their models. [11][12][13] This paper describes a one-equation reaction-kinetic model for propane-air mixture explosion in a standard 20 litre closed vessel. Moreover, results are compared with experimental data of the authors' own.

2. EXPERIMENTS

Experimental set-up

The experimental set-up is shown in Figure 1. It includes a 20-litre spherical combustion chamber which designed by principles of standard E 1226-10, and includes propane and compressed air tanks with filling devices and hoses, and further control apparatus.

The chamber is a hollow sphere with double stainless steel wall, with a volume of 20 litres. The double wall serves as water jacket to transfer the heat and to thermostatically control test temperatures. For testing, the gas in proper concentration is dispersed into the vacuumed chamber via outlet nozzle. The ignition source located in the centre of the sphere. For gases, source is electric spark, with arbitrarily changeable energy.

Pressures in the vessel during explosion were recorded with high speed pressure sensors with a frequency of 4800 Hz. The entire control unit and data acquisition unit operated on the computer with data collection function.

Gases

Propane-air mixture with 5 vol. % was used in experiments. Propane was commercially available by Linde in 99.5% purity. Air was applied from the environment for more realistic measurements. Experimental circumstances were atmospheric pressure (0 bar_g) and ambient temperature (298 K), which are specifically important in case of gases.

Experimental process

At the beginning of the filling process, the explosion chamber vacuumed to -0.2 bar_g (overpressure) with vacuum pump. After a short relaxing time for heat exchange between the air and wall of the chamber, 5 vol. % propane was injected through outlet nozzle. When the proper amount of propane gets to the sphere, the rest of the air was added through outlet nozzle, until summarized pressure of gases was equal to atmospheric pressure. Figure 2 shows schematic of propane-air loading system of the chamber.

With 60ms delay, the electric igniter was activated to ignite the mixture in the sphere. During all steps, pressure in the chamber was measured. After every experiment, chamber was cleaned to remove any remains of smoke, unburnt gases and other materials.

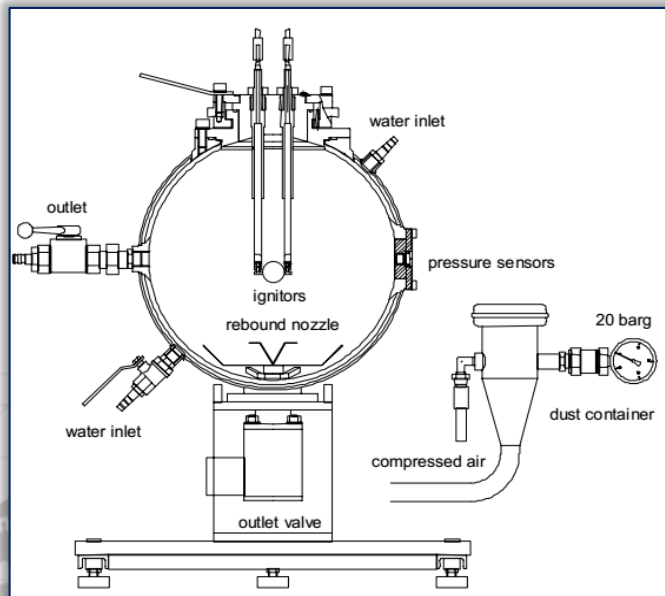


Figure 1. 20 litre explosion chamber by Kühner [14]

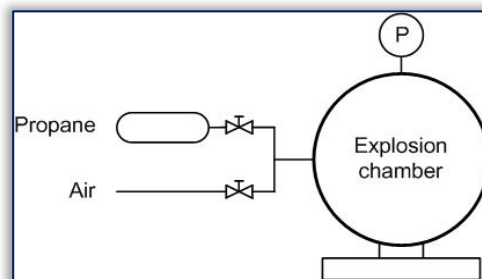


Figure 2. Schematic of the propane-air mixture loading system





3. EXPERIMENTAL RESULTS

Determined explosion characteristics of the measured explosive material were maximum explosion overpressure in case of closed chamber, and deflagration index. These are changing with fuel concentration in air, with a well-defined maximum value. In case of propane, maximum rate of pressure rise from 0 bar_g initial pressure and ambient temperature with [C₃H₈] = 5 vol. % (around equivalence ratio φ=1.2) in a cylindrical vessel can be reached [15]. Because its literature has a high amount of well written articles and books, instead of investigation of the whole concentration scale of propane-air mixtures, only 5 vol. % propane-air mixture was measured.

In closed 20-litre explosion chamber, maximum explosion overpressure was 7.75 bar, and maximum rate of pressure rise was 404.5 bar·s⁻¹. Deflagration index, K_G follows directly the cubic root equation [4][16] (Equation 2).

$$\left(\frac{dp}{dt}\right)_{\max} V^{1/3} = K_G \quad (2)$$

where (dp/dt)_{max} is maximum rate of pressure rise, V is the volume of the vessel, and K_G is deflagration index.

From the equation, deflagration index had been K_G=109.8 bar·m·s⁻¹.

4. COMPUTATIONAL ANALYSIS

Computational analysis was executed on the same mixture and volume like measurements were. The numerical model was elaborated to simulate pressure changing in the chamber during explosion process. Premixed combustion was performed with Matlab code, this model based on equation of chemical kinetics, energy conservation, heat transfer through chamber wall, and unified gas law. The kinetics of propane oxidation was modelled by a single-stage overall reaction by Equation 1, as mentioned earlier. The expression for the bimolecular reaction rate with concentration of the fuel and the oxidizer

$$r = k \cdot [C_3H_8][O_2] \quad (3)$$

where r is reaction rate, k is reaction rate constant, and further two parts of the equation is present concentration of the material.

Equation 3 was used to calculate the speed of the reaction, where reaction rate constant calculated by the following:

$$k = 7 \cdot 10^{17} \cdot p^{-0.2664} \cdot \exp(-E/(R \cdot T)) \quad (4)$$

where p is the pressure in the chamber, E is activation energy, R means gas constant and T is absolute temperature.

Equation 4 is based on expression by Frolov et al. [12], however modified in accordance with measurement results of current authors. Pressure and temperature were revised as oxidation reaction progressed. The E activation energy was 45.460 kcal·mol⁻¹ changed to proper unit.

When detailed kinetic mechanisms are used to analyse combustion, a conservation equation must be solved for each species. Differential equations of concentration changing are the following:

$$\frac{d[C_3H_8]}{dt} = -k \cdot [C_3H_8][O_2]; \quad (5.1)$$

$$\frac{d[O_2]}{dt} = -5 \cdot k \cdot [C_3H_8][O_2]; \quad (5.2)$$

$$\frac{d[CO_2]}{dt} = 3 \cdot k \cdot [C_3H_8][O_2]; \quad (5.3)$$

$$\frac{d[H_2O]}{dt} = 4 \cdot k \cdot [C_3H_8][O_2]; \quad (5.4)$$

$$\frac{d[N_2]}{dt} = 0. \quad (5.5)$$

where d[...]/dt members mean concentration change of actual material in time.

Because every single reaction draws down rising molecule number and energy release, correction of temperature needed after every step. Correction of molecule numbers were performed with proper rearranging the universal equation of energy changing without phase changing:

$$Q = c_{p,mix} \cdot \rho_{mix} \cdot V \cdot \Delta T \quad (6)$$





where $c_{p,mix}$ means average heat capacity of the mixture in the chamber, ρ_{mix} is average density of the mixture in the chamber, and ΔT is temperature-rising inside the chamber.

Heat capacity of each component depends on temperature, as the following Equation 7.1 – 7.5 describe between 200 K and 2000 K.

$$c_{p,C_3H_8} = -1.142 \cdot 10^{-6} \cdot T^2 + 4.976 \cdot 10^{-3} \cdot T + 0.399; \quad (7.1)$$

$$c_{p,O_2} = -8.083 \cdot 10^{-8} \cdot T^2 - 3.313 \cdot 10^{-4} \cdot T + 0.833; \quad (7.2)$$

$$c_{p,CO_2} = 1.100 \cdot 10^{-10} \cdot T^3 - 6.359 \cdot 10^{-7} \cdot T^2 + 1.229 \cdot 10^{-3} \cdot T + 0.531; \quad (7.3)$$

$$c_{p,H_2O} = -7.415 \cdot 10^{-8} \cdot T^2 - 7.351 \cdot 10^{-4} \cdot T + 1.636; \quad (7.4)$$

$$c_{p,N_2} = 1.075 \cdot 10^{-4} \cdot T^2 - 4.458 \cdot 10^{-3} \cdot T + 1.013. \quad (7.5)$$

For Carbon-dioxide, third-order equation fitted better than second-order ones. Average heat capacity of the mixture estimated according to Equation 8:

$$c_{p,mix} = c_{p,C_3H_8} \cdot y_{C_3H_8} + c_{p,O_2} \cdot y_{O_2} + c_{p,CO_2} \cdot y_{CO_2} + c_{p,H_2O} \cdot y_{H_2O} + c_{p,N_2} \cdot y_{N_2} \quad (8)$$

where y_i is mole fraction in gas phase, and i symbolizes each components of the reaction.

Released reaction energy was 2220 kJ/mole, and heat loss through wall of the chamber estimated by Newton's law of cooling. However, heat transfer coefficient next to the wall of the chamber and ignition temperature were unknown values. It needed to determine them with utilization of measurement data. After a short iteration progress, heat transfer coefficient was elected to $900 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$, and ignition in the chamber was performed on 1450 K temperature.

Former equations for every material were solved by ode23s built-in Matlab solver for non-stiff differential equations, which is an implementation of an explicit Runge-Kutta solver. Calculation time was 0.2 seconds with 10^{-4} second time step.

5. RESULTS AND DISCUSSION

In the calculations, the same spherical vessel and configuration was studied as experimentally. The chamber was initially filled with fully premixed 5 vol. % propane-air mixture at $p_0=1 \text{ bar}_g$ and $T_0=298 \text{ K}$. Proper amounts and material properties were known. The ignition was initiated by elevated temperature (1450 K) in every point of the volume. For it is, initial pressure in the chamber raised to approximately 4.87 bar_g , and it appears on later pressure-time functions.

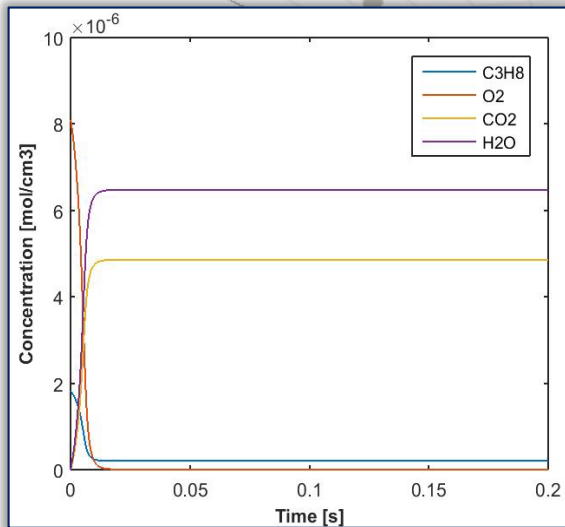


Figure 3. Concentration changes of components

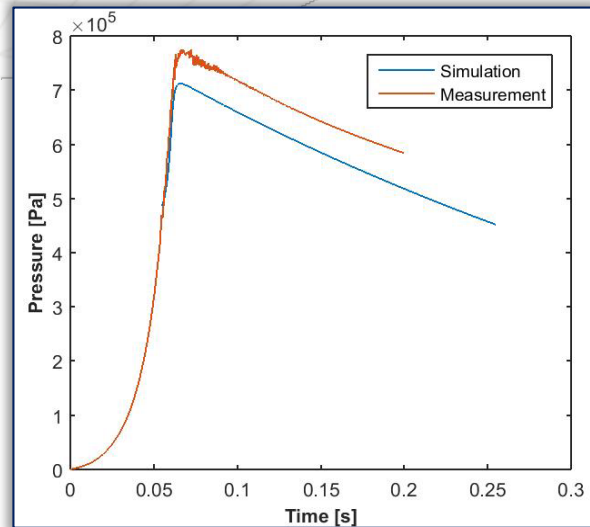


Figure 4. Pressure changes

Concentration changing histories in the vessel were recorded for every component, as it seems on Figure 3. Based on these numerically simulated curves, the corresponding pressure and temperature changing were calculated. In addition, pressure changing were stored. All of histories regarding to concentrations and pressure in every point of the volume are the same because of axisymmetry.

Figure 4 compares simulated pressure results to measured ones. A good quantitative agreement of the results can be noticed. It seems on the figure, that simulated pressures starts only approx. 4.87 bar_g , however as it earlier mentioned, this phenomenon occurred by the reason of high ignition temperature.





Maximum explosion overpressures and maximum pressure rises with deflagration indexes are shown in Table 1. As it seems, similar results published for propane explosion within 5% tolerance from the average. Thus, current measured data are acceptable as correct values, and differences could come from measurement uncertainty.

Table 1. Experimental and simulational results compared to literature

Source	p_{\max} [bar _g]	$(dp/dt)_{\max}$ [bar·s ⁻¹]	K_G [bar·m·s ⁻¹]
Measurement	7.75	404.5	109.8
Simulation	7.15	386	104.7
Razus et al. [17]	8.1	365.1	99.1
Huzayyin et al. [18]	7.2	350	95

6. CONCLUSIONS

Explosions of premixed propane-air mixtures in closed vessel were investigated experimentally and computationally. The main results are listed as follows:

- » The maximum overpressure of 5 vol. % propane-air mixture is 7.75bar_g was measured in the confined 20-litre combustion chamber. From maximum rate of pressure rise, which is 404.5 bar·s⁻¹, deflagration index was calculated in accordance with the cubic root equation. It is 109.8 bar·m⁻¹ s⁻¹.
- » Unidentified ignition temperature was determined as 1450 K
- » Unidentified heat transfer coefficient was determined next to inner wall of the cubic vessel with water jacket, as 900 W·m⁻²·K⁻¹.
- » Based on current measurements, a new numerical model has been created, which is capable to simulate concentration changes and pressure rise in a closed volume.
- » Using previously determined values, simulated maximum overpressure of the same mixture is 7.15bar_g. From maximum rate of pressure rise, which is 386bar·s⁻¹, deflagration index was calculated in accordance with the cubic root equation. It is 104.7 bar·m⁻¹ s⁻¹. These results are in good correlation in previous literatures.

More tests should be performed to evaluate the accuracy of current results. Thus, basic equations of the model will be improved, and other mixture scales will be tested. After a reliable validation process, model can be extended to vented explosion cases.

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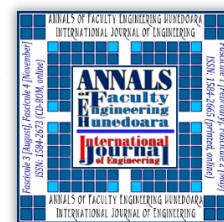




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