MultiScience - XXXIII. microCAD International Multidisciplinary Scientific Conference
University of Miskolc, 23-24 May, 2019, ISBN 978-963-358-177-3

PHENOMENOLOGICAL MODELING OF GAS EXPLOSION IN CLOSED VESSEL

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ABSTRACT

Gas explosions come out at a significant part of industrial accidents. Many of protection methods can be used to prevent them, from eliminating the causes (like disabling ignition source, displacing the oxidizing atmosphere, preventing the formation of dangerous concentrations) to suppressing the occurring explosion, and reducing damages. One type of the possibilities of protection is to reduce evolving pressure with rupture devices and vent ducts. However, their design methods are given in standards with limited equipment sizes and geometries, but further solutions are necessary in practical approaches. Derogation from recommendations of standards can only be allowed with proper technical justification. Problem can be solved with validated numerical simulations.

In this paper, a mathematical model of unvented gas-phase deflagration is presented. The model based on numerical model of Chippett (1984.) and tested against propane-air explosions at initial temperature of 293 K and initial pressure at 1 bar_a in a vessel with 0.02 m^3 volume.

Keywords: gas explosion, numerical model, Chippett model, propane

INTRODUCTION

Combustible gases and dusts occur in wide range of industrial segments from food industry, mining, pharmaceutical industry or casting to chemical plants or oil refineries [1]. One of the cheapest solutions to protect enclosures against damages of pressure rise is to install proper size of emergency vent. To design these applied elements, it is essential to know the proper explosion characteristics of the variety of combustible materials [2] and ability to treat of the enclosure. Thus, knowledge of pressure growth caused by deflagration in closed and vented vessels is essential to design and operate. [3]

DOI: 10.26649/musci.2019.047

Many of national and international standards regulate proper design of rupture devices and venting systems, but they contain such limitations which cannot be applicable to e.g. small (in Europe volume is usually less than 0.1 m^3) and large (volume is bigger than 10000 m^3) vessels, or special geometries (bends or elbows at a specified angle or radius). [4] Derogation from recommendations of standards can only be allowed with proper technical justification.

The problem can be solve with validated numerical simulations based on standard measurements. [5] In order to examine vented deflagration, it is essential to describe the process in the closed vessel. In this paper, a mathematical model of unvented gas-phase deflagration is presented. The model based on numerical model of Chippett [6] and tested against propane-air explosion measurements.

For unvented deflagrations in spherical vessels with initially quiescent mixtures which are centrally ignited, pressure rise is invertly proportional to the cube root of the volume of the vessel [7]. This equation is named as "cube root law", as the following:

$$K_G = \left(\frac{dP}{dt}\right)_{max} V^{1/3} \qquad (1)$$

where K_G is deflagration index for gases (K_{St} for a dust deflagration), $(dP/dt)_{max}$ is the maximum rate of pressure rise in closed vessel, and V is the volume of the vessel. Equation (*1*) is valid to experimental investigations, however the smaller the vessel, the wall has the more effect to the deflagration and to the K_G.

A mathematical model should be created that describes the pressure rise during explosion in a closed vessel, and correctly approximates the maximum explosion overpressure and the rate of pressure rise.

MATHEMATICAL MODEL

The mathematical model of Chippett was used with some changes and clarifications. Venting process were not studied, but the composition dependence and some limitations were incorporated into the model. The following simplifications should be considered during developing the mathematical model [6]:

1. The applied model is a premixed one, so the gas mixture is uniform in composition before the ignition, and centrally ignited.
2. The flame thickness is negligible.
3. Unburnt and burnt gases have constant specific heat ratio: 1.22 and 1.36 respectively.
4. The flame front becomes wrinkled at a critical Reynolds-number.

Governing equations

Governing equations of the model are listed hereunder. At the beginning of the process, elemental small mass has been burnt corresponding to time:

$$\frac{dm_u}{dt} = -4\pi r_b^2 \rho_u S_u \eta \tag{2}$$

where r_b is the flame radius, ρ_u is the density of unburnt mixture, S_u is the burning velocity, η is the turbulence factor due to flame wrinkling which considers the increase of flame surface.

The actual burning velocity can be estimated according to

$$S_u = S_{u0}\left(\frac{T}{T_0}\right)^{\alpha}\left(\frac{P}{P_0}\right)^{\beta}[X + \Phi] \tag{3}$$

where S_{u0} is the initial burning velocity, T and P are the actual temperature and pressure, T_0 and P_0 are the initial temperature and pressure of the gas mixture, X is a factor of turbulence increasing generated by vent opening (in unvented cases, the factor is equal with 1.0), Φ is a turbulence factor. For quiescent mixtures Φ is zero. α is temperature exponent, β is pressure exponent. In Equation (*2*), turbulence factor can be estimated as the following:

$$\eta = \left[\frac{Pr \cdot Re}{Pr_c \cdot Re_c}\right]^{\theta} \tag{4}$$

where $Pr_c \cdot Re_c$ is the flame stability parameter, θ is an empirical constant. The flame Reynolds number can be estimated as

$$Re = \frac{\rho_u r_b S_u}{\mu} \tag{5}$$

where μ is the dynamical viscosity of the unburnt mixture. Critical Reynolds number in Equation (*4*) can be estimated according to

$$Re_c = 155.555 \cdot U_c - 16.667 \tag{6}$$

where U_c is a critical expansion ratio given by $U_c = \rho_b/\rho_u$. Prandtl number Pr for all test mixtures did not vary during the tests.

$$Pr = \frac{c_p \cdot \mu}{\lambda} \tag{7}$$

where c_p is the specific heat in constant pressure and λ is the thermal conductivity of the unburnt mixture. Mass and volume conservation give Equation (*8*). Subscript 0 relates to initial mixture, u relates to unburnt and b relates to burnt mixtures.

$$\begin{aligned} M_0 &= M_u + M_b \\ V_0 &= V_u + V_b \end{aligned} \tag{8}$$

The equation of state for ideal gases is

$$PV = mR_gT \tag{9}$$

where V means the volume, m is the mass of mixture in V, R_g is the gas constant. After estimating of burnt and unburnt masses and flame radius, temperatures had been determined. From the law of isentropic gas compression, temperature of unburnt and burnt gases:

$$\begin{aligned} T_u &= T_0(P/P_0)^{(\kappa_u - 1)/\kappa_u} \\ T_b &= T_f(P/P_0)^{(\kappa_b - 1)/\kappa_b} \end{aligned} \tag{10}$$

where κ is the specific heat ratio of the burnt and unburnt mixtures. Varying temperature of the flame is assumed that

$$T_f = T_0 + 0.8(T_u - T_0) \tag{11}$$

At the end of the cycle, volumes of burnt and unburnt mixtures had been determined, and pressure of the total volume had been estimated according to the gas law (Equation (*9*)).

A computer program was written in Matlab to solve the system of equations.

Initial and boundary conditions, applied constants

Solutions of the equation systems above were compared with measured pressure histories of 5.0 volumetric % propane-air mixtures [8]. Other explosion characteristic values – e.g. maximum explosion overpressure p_{max} and deflagration index K_G were compared with another literature data [9].

Mathematical simulations performed at initial temperature of 293 K and initial pressure at 1 bar_a in a vessel with 0.02 m^3 volume. Applied time step were 10^{-6} s, from 0 s to 0.6 s.

Experimental burning velocity value for 5 volumetric % propane-air mixture were performed by Metgalchi et al. [10]. Based on their data, burning velocity of the mixture was constant during the explosion process and were equal with 0.319 m/s.

Density of the unburnt mixture above was 1.198 kg/m^3, its dynamical viscosity was $17.7 \cdot 10^{-6}$ Pas. Heat conductivity of the mixture was $2.432 \cdot 10^{-2}$ W/(mK).

Other main data which were used in the calculation in the pressure development can be seen in Table 1.

Table 1

Data used in the calculations

Data	**Value**
S_{u0}	0.319 m/s
S_u	0.319 m/s
α	2.13
β	-0.17
θ	0.25
T_f	2150 K
γ_u	1.36
γ_b	1.22

Heat transfer through the wall of the chamber were neglected, however this type of consideration will be subject of further investigations.

Some limitations have also been built into the model to describe the flame propagation process more properly. These limitations were the following:

- minimum molar number of unburnt components;
- maximum molar number of burnt components;
- maximum radius of the flame;

- minimum amount of unburnt mixture (because of mathematical considerations).

Since explosion data has been tested at a several different concentrations, stoichiometric ratio was also considered in the model, which has an effect to most of the limitations above. For the mixture of 5 volumetric % propane and air, stoichiometric ratio was 1.25, ergo this was a fuel-rich mixture.

RESULTS

First part of the investigation of the completed model was to study its behaviour in case of 5 % propane-air mixture. The characteristic of the curve, the maximum explosion overpressure and the rate of the pressure rise and deflagration index were tested against standard measurements [11] were made in a 20 litre (0.02 m^3) explosion chamber. [8] Main characteristic of the measurement and the simulated pressure rise can be seen in Figure *1*.

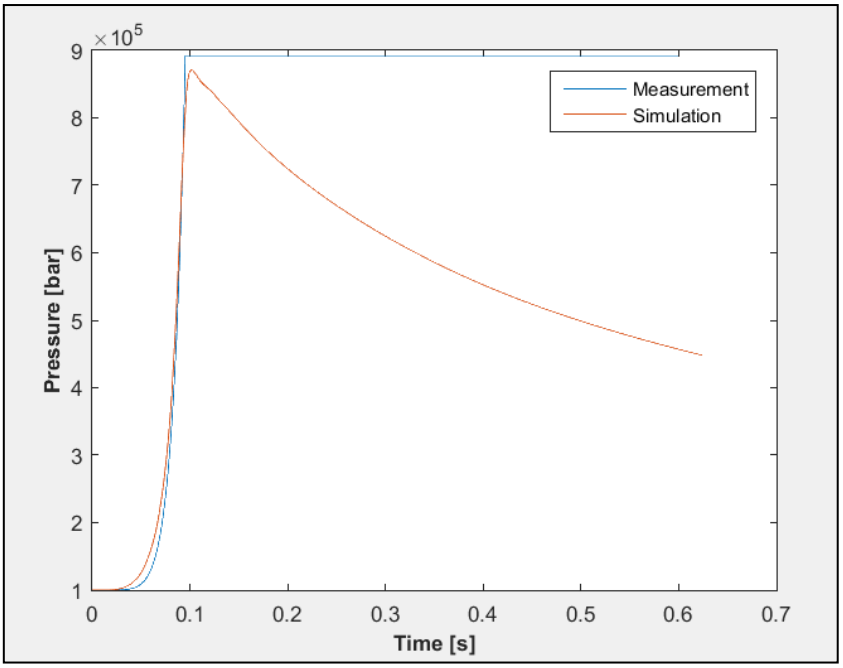

Figure 1

Pressure development in a 0.02 m^3 vessel containing 5% propane-air mixture

Table 2 illustrates a comparison of the explosion characteristics of a 5% propane-air mixture deflagration. It can be observed, that simulation give a good agreement with the measurements [8]. Deflagration index were determined according to Equation (*1*).

Table 2

Modelled results in comparison with measurement in case of 5% propane-air mixture deflagration

	P_{max} [bar_g]	$(dP/dt)_{max}$ [bar/s]	K_G [bar m/s]
Measured [8]	8,67	331,06	89,86
Simulated	8,91	308,89	83,85

Figure *1* shows that the rising phase of the modelled pressure curve follows the measurement results, but after reaching its maximum point, the two diagrams are separated. The measured curve shows a monotonic downward trend, and the simulation curve remains constant. The descending character can later be determined by considering the convective heat transfer through the wall, which is the subject of further research.

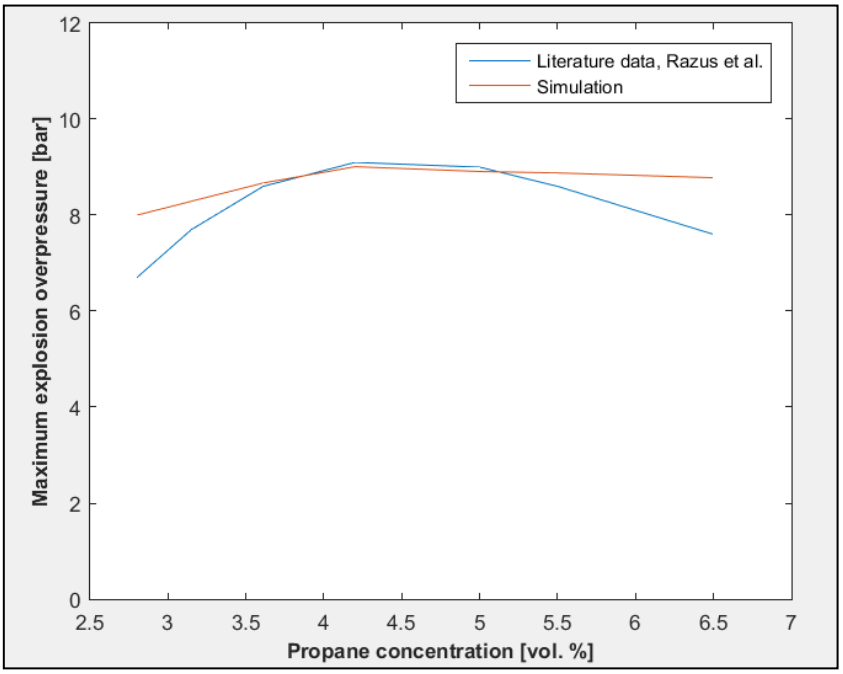

Figure 2

Maximum explosion overpressures in a 0.02 m^3 vessel containing various propane-air mixtures

As Figure *2* and Table 3 shows, the phenomenological model was made is provide satisfactory results in the middle of the concentration range, while at the ends of the range, measured and modelled values show more than 5% difference. Because of this inadequate solution, the model needs to be further refinement. It can be done by considering the variation if the flame speed as the function of pressure, temperature or concentration.

Table 3

Modelled results in comparison with literature

Propane concentration [vol %]	**P_{max} (Razus et al.)** [12] **[bar]**	**P_{max} (this study) [bar]**	**Difference [%]**
2.8	*6.7*	*8.0*	*-16.25*
3.15	*7.7*	*8.29*	*-7.12*
3.6	8.6	8.67	-0.81
4.2	9.1	9.01	1.00
5.0	9.0	8.91	1.01
5.5	8.6	8.88	-3.15
6.5	*7.6*	*8.78*	*-13.44*

SUMMARY

In this paper a mathematical model for unvented deflagrations has been described. The model based on the work of Chippett, taken into consideration the enhancement of flame surface due to wrinkling, and some mathematical limitations. The model takes account of the variation of 3.6 – 5.5 % propane-air mixture concentration range against measured and literature data.

ACKNOWLEDGEMENT

The described article/presentation/study was carried out as part of the EFOP-3.6.1-16-2016-00011 “Younger and Renewing University – Innovative Knowledge City – institutional development of the University of Miskolc aiming at intelligent specialisation” project implemented in the framework of the Szechenyi 2020 program. The realization of this project is supported by the European Union, co-financed by the European Social Fund.

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