Numerical simulation of detonation of an explosive atmosphere of liquefied petroleum gas in a confined space

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Abstract

The detonation of an explosive atmosphere from liquefied petroleum gas disseminated in air in a confined space is studied using numerical modeling with software product ANSYS AUTODYN.

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Keywords: Liquefied petroleum gas; Overpressure; Confined space; Explosion limit

1. Introduction

The liquefied petroleum gases, abbreviated as LPG, means those petroleum products which are made up of mixed variables of gaseous hydrocarbons (methane, ethane, butane) and ambient conditions, which are in a state of vapor, but can be easily liquefied. In Romania, liquefied petroleum gas, namely, petroleum product, is composed of mixture of butane (min. 90%) and propane (max. 9%) [1].

The characteristics of LPG are defined in SR 66:2007, containing mainly max. 12% C3 and min. 87% C4, and the vapor pressure is max. 7.5 bar [1].

A mixture of 8% propane and 92% butane was chosen for numerical simulation in the paper. This mixture of fuel, mixed with air, will form an explosive atmosphere. The temperatures of self-ignition and explosion limits for LPG components are presented in Table 1.

10 kg of LPG (LPG vapor) which will be subject to the detonation is used to study normal and reflected overpressures in a confined space

2. The calculation of the characteristics of LPG-air mixture using CEA program

CEA program enables the calculation of the characteristics of Chapman—Jouguet detonation. Several reports from Zack and Gordon (1960 and 1968) were intended to compare the results for the two ways of calculation of chemical equilibrium. It came to the conclusion that it comes down to the same number of equations. However, in the case of free energy minimization method each chemical species can be treated independently without having to specify a set of special effects, as it is required in the case of the equilibrium constants method [2,3].

Thus, the program that uses free energy minimization method for the calculation of equilibrium composition. The method used to obtain the parameters of engine knocking Chapman—Jouguet is described by Zack and Gordon. There are three stages in the procedure. The first stage consists in estimating the initial detonation pressure and temperature. The second stage is to use a recurrent formula for improving the parameters obtained in the first stage. During the third stage the correct values are obtained using an iterative Newton—Raphson procedure [2,3].

Table 1
Heat of combustion for various fuels [6].

Gas	Formula	Heat of combustion/ $(KJ \cdot mol^{-1})$
Propane	C_3H_8	−2219.9
Butane	C_4H_{10}	−2877.5
Isobutane	C_4H_{10}	−2869.0

The program assumes that all gases are ideal processes involved, and the interactions between the phases are neglected [8,10]. The equation of state for the gas mixture is

$$pV = nRT, \tag{1}$$

or

$$\frac{p}{\rho} = nRT, \tag{2}$$

where p is pressure (N/m²); V is specific volume (m³/kg); n is the number of moles per unit of mass mixture (mol/kg); T is temperature (K); and $R = 8314.51$ J/(mol^{-1} K^{-1}).

Based on the definition of the gas mixture, n can be written as

$$n = \sum_{j=1}^{NG} n_j, \tag{3}$$

where n is the number of moles; and is the number of moles of gas per kg of mixture.

In a conventional manner, an average molecular weight of the mixture is

$$MW = \frac{\sum_{j=1}^{NG} n_j M_j}{\sum_{j=1}^{NG} n_j}. \tag{4}$$

For iterative purposes, since are valid for the shock equations, it is necessary for these three conservation equations to be reduced to two

$$\frac{P_1}{P_2} = 1 - \gamma_{s,2}\left(\frac{\rho_2}{\rho_1}\right). \tag{5}$$

$$h_2 = h_1 + \frac{R_{\gamma_{s,2}} T_2}{2M_2}\left[\left(\frac{\rho_2}{\rho_1}\right) - 1\right]. \tag{6}$$

For ease of writing the iterative equations, symbols P^{II} and h^{II} are used to replace the right member of the above equations. These equations become

$$P^{II} - \frac{P_1}{P_2} = 0 \tag{7}$$

$$h^{II} - h_2 = 0.$$

Initial estimated temperature ratio is found by calculating the flame temperatures corresponding to enthalpy [9].

$$h_2 = h_1 + \frac{3}{4}\frac{RT_1}{M_1}\left(\frac{P_2}{P_1}\right)_0. \tag{8}$$

The initial estimates for the values $\left(\frac{P_2}{P_1}\right)_0$ and $\left(\frac{T_2}{T_1}\right)_0$ corresponding to h_2 are improved to give the following recursive formulas.

$$\left(\frac{P_2}{P_1}\right)_{k+1} = \frac{1 + \gamma_{S,2}}{2\gamma_{S,2}\alpha_k}\left\{1 + \left[1 - \frac{4\gamma_{S,2}\alpha_k}{\left(1 + \gamma_{S,2}\right)^2}\right]^{\frac{1}{2}}\right\}. \tag{9}$$

$$\left(\frac{T_2}{T_1}\right)_{k+1} = \left(\frac{T_2}{T_1}\right)_0 - \frac{3}{4}\frac{R}{M_1 c_{p,2}}\left(\frac{P_2}{P_1}\right)_0$$
$$+ \frac{R\gamma_{s,2}}{2M_1 c_{p,2}}\frac{r_{k+1}^2 - 1}{r_{k+1}}\left(\frac{P_2}{P_1}\right)_{k+1}. \tag{10}$$

$$\alpha_k = \left(\frac{T_1}{T_2}\right)_k \frac{M_2}{M_1}. \tag{11}$$

$$r_{k+1} = \alpha_k \left(\frac{P_2}{P_1}\right)_{k+1}. \tag{12}$$

where $M_2, \gamma_{S,2}$ and $c_{p,2}$ are the steady values for $\left(\frac{P_2}{P_1}\right)_0$ și $\left(\frac{T_2}{T_1}\right)_0$.

After running the CEA program, the parameters corresponding to a gaseous LPG-air mixture (Table 2) were calculated, which will be introduced into the model of material to be used in AUTODYN. The values were calculated according to the temperature of 18 °C and a pressure of 1 bar.

It can be seen from Table 2 that the maximum overpressure corresponds to a volume of 4% LPG vapor into the air. We will make the simulation of detonation for this gaseous mixture.

3. The detonation of an explosive atmosphere using modeling in Ansys Autodyn

LPG-air mixture is defined as a material using the characteristics calculated by C.E.A program. One-dimensional numerical model of this new defined material, with a predefined geometry type "wedge", for a spherical explosive cargoes in open space is shown in Fig. 1. Detonation point is in (0,0).

Table 2
Characteristics of gaseous LPG-air mixture calculated with CEA program.

% vol. LPG in the air	Detonation pressure P_D [bar] gas	Temperature of detonation $T_D/(°K)$	Speed of detonation $V_D/(m \cdot s^{-1})$	Density reagent products/initial density of gas (RHO/RHO_1)
1.5	11.850	1954.77	1457.3	1.7267
3	18.401	2786.30	1777.7	1.8090
4	19.422	2814.44	1830.2	1.7938
5	18.707	2586.47	1806.7	1.7620
6	17.644	2310.14	1754.8	1.7450