Simulation of the Dispersion of Substances Resulting from Gas Explosions

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Abstract. Directive 2014/34/EU of the European Parliament and of the Council regulates the placing on the market of equipment and protective systems intended for use in potentially explosive atmospheres. The importance of using explosion-proof equipment (certified in compliance with provisions of standards for electrical and non-electrical equipment) is crucial for avoiding catastrophic explosion-type events which may result in human victims, important material losses or may have significant consequences upon the environment. The current paper addresses a possible scenario of a pressure vessel explosion and the computational simulation and analysis of the dispersion of hazardous substances (toxic or explosive) released in the environment following the explosion-type event, in order to highlight the possible consequences. Such computational simulations may be of benefit for employers, who wish to take proactive measures in order to increase the occupational health and safety level within their activity. In this regard, results of computational simulations can be integrated by the companies in the development of emergency response plans, aiming at minimizing the hazardous effects of the releases of toxic/explosive gases upon the workers and surrounding atmosphere.

1. Introduction

The explosion risk is one of the most important industrial risks, being present in all units that produce, use, handle, store or transport hazardous substances, respectively products with flammable and explosive properties. The use of electricity in potentially explosive atmospheres has many peculiarities due to which the problems raised by the design, construction and operation of electrical equipment and installations present many difficulties, their approach requiring special attention in considering multiple technical, economic, occupational safety and environmental protection aspects.

The selection process for electrical equipment used in technological installations operating in explosive atmospheres must comply with the essential safety and health requirements regarding explosion protection specified in the ATEX Directive 2014/34/EU (for equipment and protective systems intended for use in potentially explosive atmospheres), as well as to comply with other industry standards [2, 3].

In industrial installations where flammable or combustible substances are processed, used or stored, an explosive atmosphere may occur, generating an explosion hazard. In this regard, in order to ensure explosion protection, the electrical equipment used in such installations must be chosen correctly so that to ensure a proper OHS level and to prevent it from becoming a source of ignition for the explosive atmosphere.
In this respect, the characteristics of all parameters involved in the generation of an explosion and those related to the safety of electrical equipment intended for use in potentially explosive atmospheres generated by flammable gases, vapors or dusts must be highlighted. The process of selecting electrical equipment intended for use in such atmospheres is quite complex, involving a thorough knowledge of these parameters [4].

2. Generalities on explosion protection
2.1. Basic concepts on the occurrence of potentially explosive atmospheres

Explosion prevention and explosion protection are of major importance for occupational health and safety, in order to minimize losses (both human and material). Explosive atmosphere is defined as a mixture with air, under atmospheric conditions, of flammable substances in the form of gases, flammable vapors or combustible dusts, in which, after ignition, combustion spreads throughout the unburned mixture. To generate an explosive atmosphere, the flammable substance must be present in certain concentrations. If the concentration of explosive substance in the air is too low or too high, no explosion may occur. Therefore, the explosion can only occur if there is a source of ignition and only if the concentration falls within the explosive range of the substance, ie between the lower explosive limit (LEL) and the upper explosive limit (UEL). The explosion limits of the substance may depend on the pressure, oxygen concentration in the air and temperature. The mechanism of an explosion generated by a mixture of flammable gas, vapor or air mist can be expressed by the well-known explosion triangle shown in figure 1. Thus, the occurrence of an explosion is conditioned by the simultaneous presence of the following three factors:

- presence of fuel (flammable gases, vapors, dust / powders);
- presence of oxidizer (oxygen, oxidizing substances);
- efficient source of ignition to ensure the activation of molecules in order to ignite and propagate the fast combustion reaction.

![Figure 1. Explosion triangle](image)

2.2. Equipment selection criteria

The correct selection of electrical equipment for hazardous areas requires a variety of information, such as:

- classification of the hazardous area (including, if necessary, the classification of gases and vapors in relation to the group or subgroup of electrical equipment) [3];
- temperature class or ignition temperature of the gases or vapors involved (in the case of explosive atmospheres generated by flammable gases, vapors, mists) [2];
- the minimum ignition temperature of the flammable dust cloud, the minimum ignition temperature of the flammable dust layer and the minimum ignition energy of the flammable dust cloud (in case of explosive atmospheres generated by combustible dusts);
- external influences and ambient temperature.

All equipment operating in explosive atmospheres has to be designed in such a way that it cannot ignite the explosive atmospheres for which it is designed to operate.
2.3. Use of computer simulations for decreasing the explosion risk

The approach a possible explosion scenario, simulation and computational analysis of the dispersion of hazardous substances (toxic or explosive) released into the environment following a potential event is necessary for highlighting the possible consequences. Such numerical simulations can be useful for proactive and predictive measures for increasing the OHS level for the assessed activities. In this regard, the results of computer simulations can be integrated into the development of emergency response plans aimed at minimizing the hazardous effects of toxic / explosive gas emissions on workers and the surrounding atmosphere [7].

A software package used in the analysis of explosion phenomena and their consequences is CFD software. The CFD (Computational Fluids Dynamics) tools used to perform computer simulations in this paper are applications for the various steps presented above and are an integral part of the ANSYS multiphysics package. This CFD package is a comprehensive tool for multiphysics analysis, which allows the user to combine the effect of two or more physical phenomena (structural, thermal, electrical, magnetic, electromagnetic, electrostatic, fluid flow) [5, 6].

The following applications from the package were used:

- ANSYS Design Modeler - provides modeling tools specific to the simulation requirements, including tools for designing the geometric model and the possibility to modify the existing geometry;
- ANSYS Meshing – develops the mesh of virtual geometries and provides very complex pre / post-processing tools, with direct connection to solvers. The product provides a direct link from CAD programs to pre / post - CAE processing;
- ANSYS FLUENT - is a flexible CFD application, used for simulations of any complexity. Offers a full range of physical models that can be used for a wide range of applications, from various industries.

3. Materials and methods

The study presented within the paper analyzes the case of an explosion generated by methane gas inside a production room, highlighting the effects of hazardous substances resulting from the explosion. In consequent studies there will be taken into account the simulation and highlighting of hazardous substances resulting from explosions on the LPG and CNG storage and supply containers. At the same time, following the simulations performed from the CFD program, the mechanical effects of the structures and also on the objects (technical installations, equipment, vehicles, etc.) located in the immediate vicinity of the explosions can be determined.

CFD applications are tools for computerized simulation of physical processes through mathematical models and numerical solutions based on physical principles and functions with assumed accuracy, resulting in values of selected variables that, through post-processing, contribute to the construction of graphs, vector fields, color icons, to give the user the most representative images of the studied phenomena [1]. All these, gathered behind the CFD application, represent the so-called blackbox. The user enters the input data, which is processed in the blackbox, after which the results are provided. Entering erroneous input data will lead to erroneous results (Figure 2).

![Figure 2. CFD blackbox](image)

Commercial CFD packages include modules for designing geometric spaces, building mesh networks, flow simulation and post-processing. Solving problems using CFD techniques involves defining several steps, as presented in figure 3.
3.1. Chemical reaction of methane combustion

Chemical reactions involve the transformation of one or more substances into different substances. In other words, chemical reactions produce a rearrangement of atoms or ions to form substances other than those initially involved in the reaction.

Chemical equations are used to describe chemical reactions, showing, on the one hand, the substances that react - called reactants - and, on the other hand, the substances formed - called reaction products. The chemical equations also define the quantities of substances participating in the reaction.

The equation that describes the reaction between methane gas and oxygen is presented below:

$$\text{CH}_4 + 2 \text{O}_2 = \text{CO}_2 + 2 \text{H}_2\text{O} \quad (1)$$

Methane gas reacts with oxygen to generate carbon dioxide and water. Moreover, it follows from equation (1) that for each molecule of methane two molecules of oxygen are needed for the reaction to take place, resulting in one molecule of carbon dioxide and two molecules of water (figure 4).
The chemical balance of the equation, achieved by the stoichiometric coefficients, must always include the same number of each type of atoms, on each side of the equality. From the above it can be seen that the chemical equation of oxidation of methane satisfies the law of conservation of mass. The chemical equation describes the fractions participating in the reaction, ie the molar fractions of the reactants and reaction products, as well as their relative masses.

3.2. Graphical representation of the methane oxidation reaction
Transposing in a graphic application the combustion reaction of methane in the presence of oxygen, we obtain the decomposition curves of methane gas, respectively of carbon dioxide production (figure 5). The graphics were made through the Reaction Kinetics Live application, offered in the demonstration version by Flextron BT Hungary.

![Figure 4. Methane oxidation reaction](image)

3.3. Reaction mechanisms of methane oxidation
The FLUENT application in the ANSYS multiphysics package offers, through the built-in database, two mechanisms for methane oxidation. The first mechanism consists of the basic reaction:

\[
\text{CH}_4 + 2\text{O}_2 \Rightarrow \text{CO}_2 + 2\text{H}_2\text{O}
\]

The second mechanism is the one developed by Westbrook and Dryer (WD1), differing from the first only in that the reversible reaction of carbon monoxide oxidation is integrated into the program by two irreversible reactions:
\[ \text{CO} + 0.5\text{O}_2 \Rightarrow \text{CO}_2 \]  
\[ \text{CO}_2 \Rightarrow \text{CO} + 0.5\text{O}_2 \] 

(3) 
(4)

In addition to the mechanisms comprised within the database, files in CHEMKIN format (software dedicated to chemical kinetics) can be imported into the FLUENT app, describing mechanisms such as GRI-Mech or even other ones developed by the user.

3.4. Reactants consumption and formation of reaction products

Based on the result generated by the computer simulation - the graph of the decomposition of methane in the oxidation reaction was developed (figure 6) for the considered monitoring point.

![Figure 6](image)

**Figure 6.** (a) Methane decomposition and reaction rate, time functions; (b) Fuel consumption and end of reaction

As can be seen from figure 6 a) and b), once with the consumption of the combustible material in the air-methane mixture, the reaction rate decreases proportionally, the reaction ending after reaching the zero value of the methane concentration. In contrast to the decrease in reaction rate, as the reaction develops, reaction products are generated, namely carbon dioxide and water, their concentrations increasing in accordance with the decrease in the concentration of the reactants. Figure 7 shows the graphs of production / decomposition of carbon dioxide / methane.

![Figure 7](image)

**Figure 7.** Production / decomposition of carbon dioxide / methane
4. Results and discussions
For the exposure, analysis and validation of the simulation is considered a room which has the following dimensions 12x30x7m and whose designed geometry is presented in figure 8 a). Through the meshing process, the fluid volume representing the interior of the room was divided into 105702 finite volumes, as shown in figure 8 b.

![geometry of the analysed room](image1)

(a) geometry of the analysed room

![mesh result](image2)

(b) mesh result

The input data for the set room volume concentrations required for the simulation are shown in Table 1

| Component | Concentration | Molar Mass | Comp. mass | Mass Fraction |
|-----------|---------------|------------|------------|---------------|
| CH4       | 9.5           | 16.04246   | 152.40337  | 0.055         |
| O2        | 18.95975      | 31.9988    | 606.6892483| 0.220         |
| N2        | 71.54025      | 28.0134    | 2004.085639| 0.725         |

Following the running of the simulation regarding the development of the explosion process, in figure 9 are represented the color contours of the temperatures distributed in the analyzed volume, respectively the propagation of the flame front inside the room.
During the methane combustion process, the reactants experienced a decrease in the average concentration over the entire analyzed volume shown in Figures 10 - 13.

**Figure 9.** Flame front propagation and temperature variation inside the room

**Figure 10.** Average molar fraction of methane over the entire volume
The volumetric concentration of the reactants / reaction products is calculated by multiplying, by 100 times, the molar fraction.

5. Conclusions

Following the simulation analysis, the following conclusions can be drawn:

- The possibility of a reaction to take place over a period of time is studied in chemical kinetics, a field that provides details about the reaction rate, the number of molecules actually involved in the reaction and the intermediate stages of chemical transformation.
- The reaction rate is the number of molecules that react in a unit of time.
In order to describe the reaction rate, it is necessary to determine the concentration of a reactant or product, at successive intervals, during the reaction.

The reaction rate is directly proportional to the concentration of the reactant and its reaction order.

Chemical reactions have uneven velocities over time. The reaction rate is higher at the beginning, when the reactant concentrations are maximum; it decreases first rapidly, then more and more slowly, as the reactant concentrations decrease, tending asymptotically to zero, when the reactant concentrations become very low.

The reaction rate can be represented by the derivative of the decrease of the concentration of one of the reactants, or by the derivative of the increase of the concentration of one of the reaction products.

The activation energy is the excess energy, relative to the average energy of the gas molecules, that the reactant molecules must possess in order to react. Molecules do not react unless they together have an energy greater than or equal to the activation energy.

An increase in temperature corresponds to an increase in the reaction rate for the same values of the activation energy and the concentrations of the chemical species involved in the reaction.

The chained reactions that characterize an explosion phenomenon can be defined by three stages: initiation, propagation and interruption. They define a reaction mechanism.

The use of computer simulations is particularly important for avoiding catastrophic events caused by explosions that can lead to human casualties, significant material loss or have significant consequences for the environment. Moreover, the presented simulation addresses a possible scenario of an explosion of methane gas inside a production room and the calculation analysis of the dispersion of hazardous substances (toxic or explosive) released into the environment so that to highlight the possible consequence but also for establishing the causes which led to the ignition and propagation.

References

[1] C. Baxevanou, D. Fidaros, D. Papanastasiou, T. Bartzanas, C. Kittas, “Numerical simulation of internal microclimate inside a livestock building”, Environmental Engineering and Management Journal, vol. 16, pp. 2513-2523, 2017.

[2] EU Directive, Directive 2014/34/EU relating to equipment and protective systems intended for use in potentially explosive atmospheres, Official Journal of the European Communities, L 96/351, 29.3.2014.

[3] EN Standard, EN Standard 60079 Explosive atmospheres - Part 10-1: Classification of areas - Explosive gas atmospheres, 2009.

[4] V.M. Pasculescu, E. Ghicioi, M. S. Morar, D. Pasculescu, M. C. Suvar, “Computational study for improving the quality of safety measures for LPG filling stations”, Quality - Access to Success, vol. 20, pp. 25-30, 2019.

[5] N. I. Vlasin, C. I. Colda, V. M. Pasculescu, D. Pasculescu, D. Fotau, “Turbulence modelling in computational simulation of methane explosions”, Proc. of 6th International Multidisciplinary Scientific Geoconference (SGEM), Science and Technologies in Geology, Exploration and Mining, Vol. II, pp. 965-972, Albena, Bulgaria, 2016.

[6] N. I. Vlasin, C. Lupu, E. Ghicioi, E. Cozma, V. Arad, “Numerical analysis of the ignition of air-methane explosive mixtures related to underground mining atmospheres”, Proc. of 13th International Multidisciplinary Scientific Geoconference SGEM 2013, Albena, pp. 563-570, 2013.

[7] D. Wang, X. M. Qian, M. Q. Yuan, T. C. Ji, W. Xu, S. Liu, “Numerical simulation analysis of explosion process and destructive effect by gas explosion accident in buildings”, Journal of Loss Prevention in the Process Industries, vol. 49, pp. 215-227, 2017.