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NEW TOOLS FOR ESTIMATING THE EXTENT OF HAZARDOUS AREAS GENERATED BY GAS LEAK EXPLOSIONS

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Abstract

The current paper is an overview on previous and ongoing research carried out by the authors concerning the use of Computational Fluid Dynamics for the accurate classification of hazardous Ex areas generated by flammable gases, for the optimization of computational simulation of air-methane mixture explosions by using ANSYS CFX and FLUENT and for calibrating computational simulations of gas explosions using the Schlieren effect. These research works containing analytic studies have led to the observation of basic principles which come to support the benefit of computational approaches for estimating gas dispersion within technological installations in which are handled or stored flammable materials and in which there are likely to occur explosive atmospheres. Preliminary results have led to the idea of developing a computational method for assessing the hazardous area extent in case of gas leak explosions in confined spaces. The computational method intended to be developed has to be validated in the lab using an experimental chamber as domain for analysing accidental flammable gas leaks from transportation installations and for studying the formation, ignition and burning of air-flammable gas mixtures in confined spaces. Results obtained from physical experiments will be used for calibrating the mathematical models. Further, verification and validation of computational simulations carried out based on physical experiments will be performed by a comparative analysis of virtual results with the experimental ones. In the end, the mathematical model will be implemented on a small-scale reproduction of a confined industrial area with explosion hazard.

Key words: computational method, confined space, explosion, extent, gas leak, hazardous area

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1. Introduction

The starting point of the current research is represented by previous works (Pasculescu et al., 2014a), in which computational simulations of flammable gas leaks into a confined space were performed, using Computational Fluid Dynamics (CFD) simulation software. Nationally, this type of approach which makes use of CFD techniques for assessing the extent of hazardous areas are in early stages. From our knowledge there are no other Romanian works performed in this direction. Moreover, computational simulations of flammable mixtures explosions are performed only by the National Institute for Research and Development in Mine Safety and Protection to Explosion – INSEMEX Petroşani (INCD INSEMEX Petrosani) and they represent the basis for several national research projects (Vlasin, 2015a, 2015b, 2017; Vlasin et al., 2015).

The Australian standard AS/NZS 5601.1:2013 postulates the fact that there is no allowable leakage rate for Liquefied Petroleum Gas (LPG) installations or for natural gas installations with a metering pressure or operating pressure of 2.75kPa or above. Such installations, whether new or existing, mustn't have any pressure losses when tested to the requirements of this standard. Such regulations on

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handling flammable substances are present worldwide. ISO/TS 16901:2015 stipulates the basic methodology and provides directions to those who perform evaluation of the safety level as a feature of the design and operation of liquefied natural gas installations. In the European Union, the legal framework has just changed, introducing the new Regulation (EU) 2016/426 on appliances burning gaseous fuels, fully applicable as of 21 April 2018 and replacing the old Directive 2009/142/EC relating to appliances burning gaseous fuels.

In Romania, hazardous areas generated by flammable gases are classified into zones according to European Norms in force (EN Standard, 2009). The causes of accidental leakages can be external or internal corrosion, internal erosion, equipment wear, metallurgical defects, operator errors or third party damage (Nolan, 1996). Gas leakages are studied all over the world, from the estimation of gas leak rates through very small orifices and channels (Bomelburg, 1977) to computational simulations (Xuegang et al., 2012).

Taking into account that predicting the emission and dispersion of flammable gases is of high importance in terms of process safety (Alves et al., 2019), researchers worldwide are using mathematical models, developed within open-source or commercial software, for investigating the extent of hazardous areas generated by flammable gases or vapours, on the grounds of thermodynamics and based on experimental observations (Fiates et al., 2016; Ordouei et al., 2018; Pasculescu et al., 2017; Souza et al., 2019).

Computational simulation of flammable gases and vapours has significant practical implications, allowing not only visualization, but most important the improvement of the quality of conclusions drawn up during the hazardous area classification (Krauze, 2018; Pasculescu et al., 2019a). On the other hand, flammable mixtures explosions have been also studied from ignition (Werle and Wilk, 2010), to the propagation of the shock wave (Bedarev et al., 2004) and flame front, bringing along results for pressure levels which are hazardous for the human lungs or ears, as well as for the sensitivity of the human body to thermal radiation etc.

Computational studies of flammable mixtures explosions generally aim to provide guidance on the required strength of various industrial assets (equipment, walls, buildings etc.) or to verify a certain design (Hansen et al., 2016). Not only the industrial sector is of concern for researchers, accidental gas explosions in civil buildings being also investigated using computational means. The simulation results are compared with the actual imprint of the shock wave propagation within the buildings concerned (Baxevanou et al., 2017). Such studies can provide guidance on the assessment of injuries and damages and can help develop new building designs, which to be safer, in terms of explosion pressure discharge (Wang et al., 2017).

The novelty of the paper is represented by the fact that it deals with a research study combining scientific and technical investigations on flammable gas leaks, formation of explosive atmospheres and their ignition, development of explosions in confined spaces of complex geometry and the analysis of effects of pressures resulting with regard to explosion protection. Previously mentioned aspects are of significant concern and have been investigated separately by important scientists worldwide. However, the current article, by combining all these issues into a whole, represents a novel approach for the complex field of computational investigation of gas leaks and resulting explosions.

2. Objectives

The overall objective of the proposed research consists in the development of a computational method for assessing the hazardous area extent in case of gas leak explosions occurred in confined spaces. In order to achieve this goal, several specific objectives shall be addressed, namely:

- to develop an experimental stand used as domain for analysing accidental flammable gas leaks from transportation installations and for studying the formation, ignition and burning of air-flammable gas mixtures in confined spaces. The assembly shall comprise a confined space, an installation for transporting flammable gases (a fissure being simulated on its' path), possible process installations, source for igniting the explosive atmosphere, equipment specific for Schlieren techniques, pressure transducers connected to an oscilloscope for determining pressure values in various points of the confined space, representing the small-scale reproduction of an industrial area with risk of explosive area occurrence;
- to obtain data sets on the formation of explosive mixtures generated by gas leaks, on their ignition and on their combustion. These data sets (pressures, velocities and video recordings on the behaviour of the flame front) will be obtained from physical experiments focusing on two cases of explosive atmosphere occurrence: one in which the analysed area comprises only the flammable gas transportation pipe, and the other one for the case in which the analyzed area comprises also industrial flammable gas consumption installations;
- to test, select and calibrate mathematical models which are proper for simulating gas leaks and explosions of flammable atmospheres;
- to perform and validate the computational simulations.

Computational simulations are going to be performed using ANSYS Fluent which is specialized for fluid flow analyses. The verification and validation of computational simulations carried out based on physical experiments will be performed by a comparative analysis of virtual results with the experimental ones. Moreover, even if a high similitude results after the analysis, the dependence of the solution on the resolution of the mesh will be tested.

Taking into account the above mentioned, the objectives of the research are well correlated with the outcome, leading to the extension of knowledge about the explosion type phenomenon, and later at increasing the occupational health and safety level, the data obtained being used for developing measures and solutions for protection to explosion (Buica et al., 2016; Jurca et al., 2014; Lupu et al., 2017).

3. Experimental

3.1. Method description

Associated to the current theme, there have been obtained promising preliminary results from previous research (Pasculescu et al., 2013, 2014a, 2014b, 2015, 2015a) aiming the following:

- the use of computational simulation technologies for analysing flammable gas dispersion in industries in which may occur flammable atmospheres, in order to integrate these modern techniques into the process for hazardous Ex areas classification and to improve the currently used methods for determining the parameters which characterize hazardous areas generated by a release source (Prodan et al., 2016; Szollosi-Mota et al., 2012). There have been modelled accidental leaks which may occur within a technological installation and which may generate hazardous gas releases leading to the formation of an explosive atmosphere. CFD techniques were used for simulating fissures (of different diameters) in flexible fittings from within a technological installation in which are used flammable gaseous substances, in order to analyse the dispersion of gases released through these fissures.

There have been monitored the total times from the occurrence of the leak up to the reach of concentrations representing 25% (Fig. 1), respectively 50% LEL (Lower Explosion Limit). Fig. 1 presents the total time for reaching 25% LEL (monitored within the complete domain), of cubic shape, having a volume of 8 m^3, the initial conditions for this case being summarized in Table 1.

Table 1. Initial conditions for problem setup

Parameter	***Value***
Average atmospheric pressure	101325 Pa
Absolute pressure inside the domain	104325 Pa
Molar weight of the gas	19.29 g/mol
Gas density	0.789 kg/m^3
Gas velocity at discharge	113.103 m/s
Temperature	298.15 K
Discharge orifice area	1 mm^2

The results obtained have validated the approaches for estimating gas dispersions through computational methods and confirmed that CFD techniques represent an extremely useful tool for their analysis in case of installations in which are handled or stored flammable materials and in which exists an explosion hazard.

- to create subroutines in C programming language, which to represent extensions of the standard tools included within ANSYS Fluent. These subroutines are useful both in the mathematical approach of fast combustion phenomenology, as well in investigating explosion type events resulting in material damages and human losses, in assessing the explosion risk within work/technological processes carried out in explosive atmospheres.

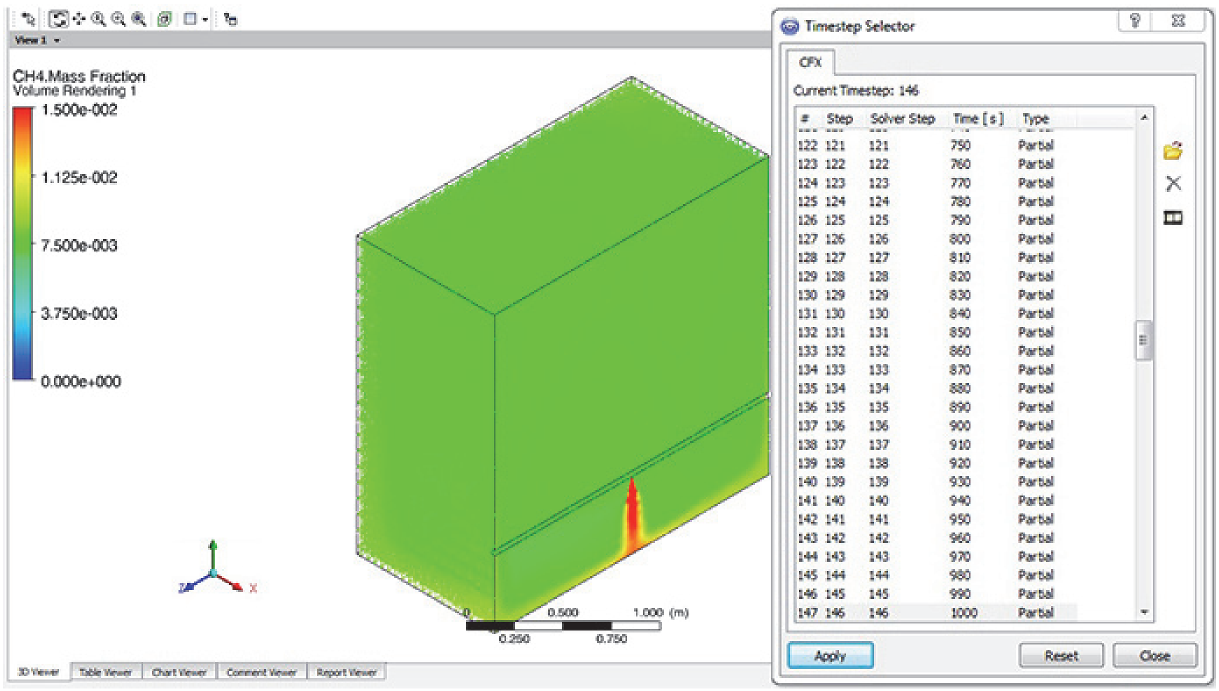

Fig. 1. Reach of a 25 % LEL concentration - mass fraction 0.0075 (1 mm^2 fissure)

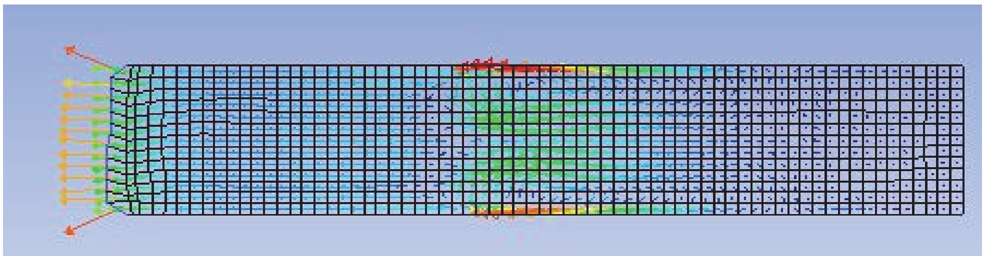

Fig. 2. Wall breaking moment

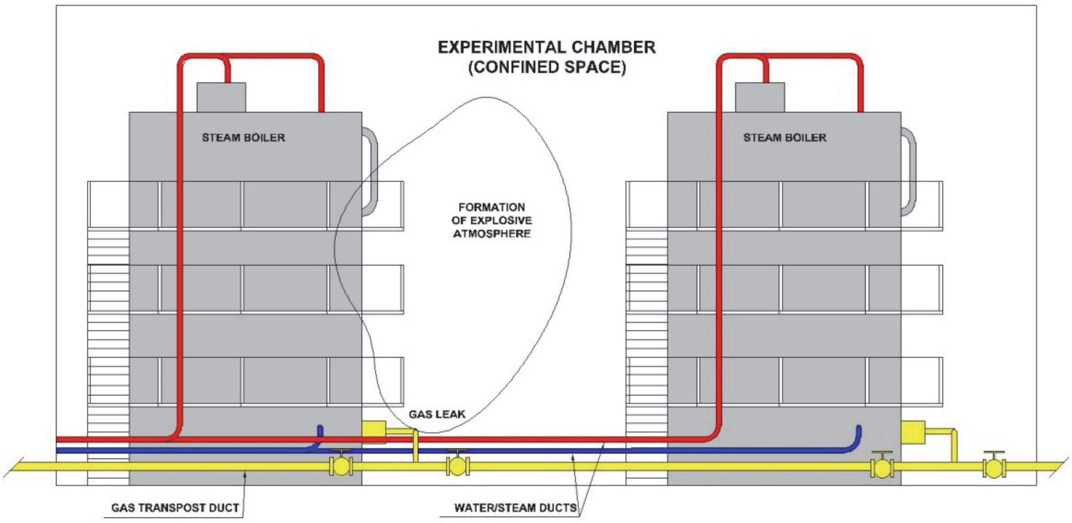

Fig. 3. Principle diagram of the experimental chamber

Also, computational simulations of stoichiometric air-methane mixture explosions within a confined space have been performed. For verifying the applicability of the model (in case of an explosion occurred within a confined space, three different situations have been taken into account (Cioclea et al., 2015; Pasculescu and Niculescu, 2015; Pasculescu et al., 2019b): i) confined space explosion, without wall deformation; ii) confined space explosion, with one wall deformation, but without breaking it; iii) confined space explosion with one wall deformation and its' breaking. Pressure vectors contours resulting from post-processing are presented in Fig. 2.

A normal behaviour of pressure and velocities gradients on the analysed domain resulted in a pressure increase up to the deformation and breaking of the wall, afterwards decreasing and tending to balance with the pressure from outside the domain. By comparing the results of the simulations, the dynamic mesh method has been proven to be suitable for modelling explosions in confined spaces.

Research projects which led to the basic concept of the project are presented in detail in Pasculescu (2014), and Vlasin (2015a, 2015b, 2017). Physical experiments on gas leak explosions in confined spaces are intended for studying the formation, ignition and burning (Darie et al., 2017) of air-flammable gas atmospheres generated by gas leaks in confined spaces. In order to achieve these, there will be developed and instrumented an experimental test stand. The experimental stand used as domain for analysing accidental flammable gas leaks from transportation installations and for studying the formation, ignition and burning of air-flammable gas mixtures in confined spaces has to fulfil the following conditions: i) to comprise a confined space (experimental chamber – Fig. 3), with transparent walls, equipped with an installation for transporting flammable gases (on its' path being simulated a fissure) and with possible process installations existing in the proximity of the gas transportation system, representing a small-scale reproduction of an industrial area with explosion hazard. The installation presented schematically in Fig. 3 is hypothetical and reproduces in principle such a hazardous area; ii) to comprise a source for igniting the explosive atmosphere occurred in the confined space, following the gas leak from the simulated fissure; iii) to comprise equipment specific for Schlieren techniques, for the high-speed video-recording of the phenomena of flammable gas leaking through the fissure, of gas dispersion and formation of the explosive atmosphere on one hand, and on the other hand the propagation of the pressure wave and flame front; iv) to be equipped with pressure transducers connected to an oscilloscope, for determining the pressure values in various points of the confined space.

Physical experiments focus on two cases of explosive atmospheres occurrence: i) the analysed area comprises only the flammable gas transportation pipe; ii) the analysed area comprises the flammable gas transportation pipe and industrial flammable gas consumption installations.

By comparing the two cases there is followed to notice the influence of geometric elements on the propagation of the shockwave and flame front and to highlight differences in pressure values monitored in homologous points located on the boundaries of the experimental chamber. The flammable gas transportation through the system will be monitored using a flow-meter so that, by knowing the section of the fissure, in order to determine the quantity of gas leaked from the transportation system into the analysed confined by applying the mass flow equation (Eq. 1):

$$\frac{dG}{dt} = S\sqrt{\gamma\frac{M}{RT}\left(\frac{2}{\gamma+1}\right)^{(\gamma+1)/2(\gamma-1)}} \qquad [g\cdot s^{-1}] \qquad (1)$$

where: S – fissure section [mm^2] ; γ – polytropic index of adiabatic expansion; M – molecular weight of the gas from the pipe [g/mol]; R – universal gas constant [J·mol^{-1}·K^{-1}]; T – absolute temperature inside the pipe [K]; t – time [s].

The transparent walls of the experimental chamber provide its' integration into a configuration for visualising the Schlieren effect (Fig. 4). The Schlieren technique is an optical method used to observe refractive index gradients in gases, especially air, and other clear media. The dispersion of flammable gases within the studied volume and the formation of explosive atmosphere will be recorded using a video camera, to the viewing limit by Schlieren effect of the densities variations generated by the leak. By using a repetitive spark generator, with programmable supply (Fig. 5), electric sparks will be generated at certain time steps, thus determining the period between the moment of gas leak occurrence and the moment when the formed explosive atmosphere ignites. This time period will be determined also in case of modifying the location of the spark, depending on the distance between the gas source and the ignition source.

The fast combustion process will be recorded using a high-speed camera, by applying Schlieren techniques (Fig. 4). These recordings allow the determination of velocities between any two points located within the domain and, moreover, of the behaviour of the flame front by highlighting temperature gradients from the limit between burned and unburned gases (Vlasin et al., 2013). An image of the flame front recorded in experiments performed at INCD INSEMEX Petrosani on methane explosions in rectangular tubes in presented in Fig. 6.

The advantage of these combined techniques in case of monitoring velocities is represented by the possibility to determine values between any two points located very close to each other, resulting in a much more detailed graph of the burning process evolution compared to test stands with opaque walls, in which velocity values are obtained only as average between two locations of the transducers.

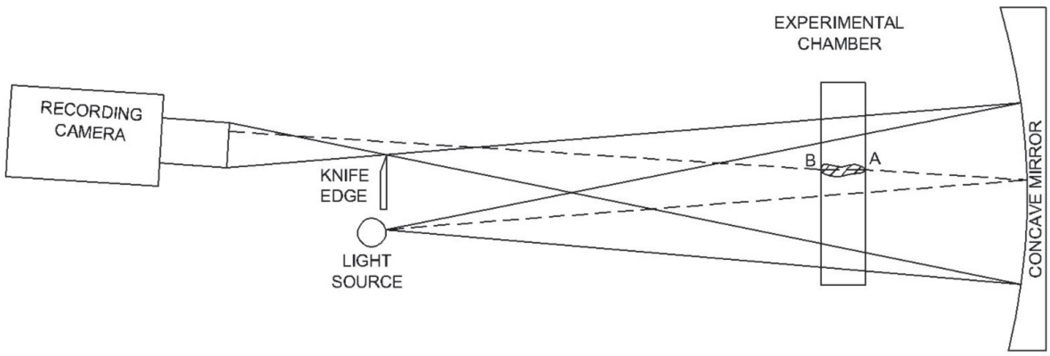

Fig. 4. Schlieren setup principle

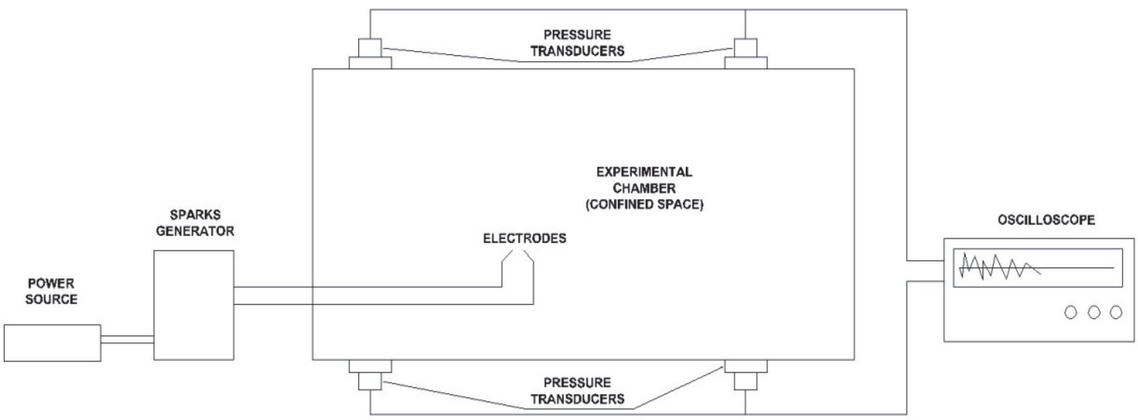

Fig. 5. Experimental chamber fitting

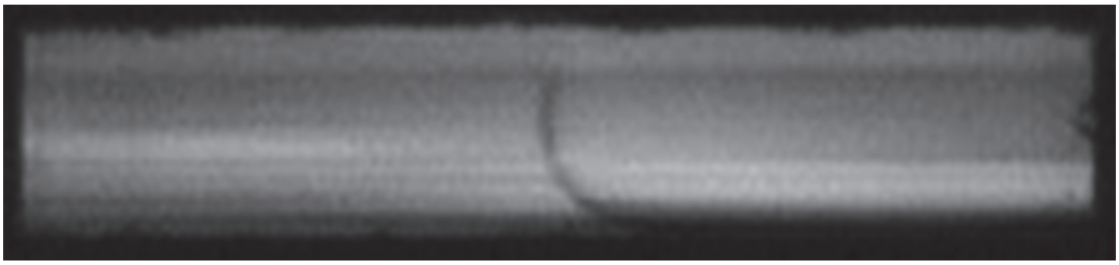

Fig. 6. Flame front image obtained by Schlieren techniques

Pressure levels will be recorded using transducers mounted at certain distances from the explosion ignition location, within the transparent walls of the experimental chamber (Fig. 5). Results obtained will consist in datasets (pressures, velocities and video recordings on the behaviour of the flame front) corresponding to the two previously mentioned cases and to the distance between the gas source and the ignition source.

Computational simulation of gas leak explosions occurred in confined spaces aim to achieve a valid mathematical model which can be used for modelling gas leak explosions occurred in complex confined spaces.

3.1.1. Numerical model calibration

Computational simulations will be performed using ANSYS Fluent which is specialized for fluid flows. The first requirement for the success of a computational simulation is the development of the virtual geometry so that to strictly respect the real space, in this case the constructive characteristics of the experimental chamber.

Meshing the virtual geometry in control elements is also of high importance: a small number of elements will result in a low resolution of the mesh network. The mesh method applied and the resulting mesh generated have to provide the possibility for the simulation to fulfil a very important requirement, namely the error bars generated by meshing have to be acceptable. A correct mesh usually generates proper simulations, decreasing local and global errors below the established levels. ANSYS Fluent disposes of a solver which is based on pressure, therefore convection and diffusion elements are composing at inlets the net transport of species.

To solve conservation equations for chemical species, ANSYS Fluent predicts the local mass fraction of each species, *Yi* (dimensionless quantity), through the solution of a convection-diffusion equation for the i^{th} species. This conservation equation takes the following general form (Eq. 2):

$$\frac{\partial}{\partial t}(\rho Yi) + \nabla \cdot \left(\rho \overrightarrow{vYi}\right) = -\nabla \vec{Ji} + Ri + Si \qquad (2)$$

where *Ri* is the net rate of production of species *i* by chemical reaction and *Si* is the rate of creation by addition from the dispersed phase plus any user-defined sources.

An equation of this form will be solved for N^{-1} species where *N* is the total number of fluid phase chemical species present in the system. Since the mass fraction of the species must sum to unity, the N^{th} mass fraction is determined as one minus the sum of the solved mass fractions. To minimize numerical error, the N^{th} species should be selected as that species with the overall largest mass fraction, such as when the oxidizer is air. In Eq. (2), *Ji* [mol·m^{-2}·s^{-1}] is the diffusion flux for species *i*, which arises due to gradients of concentration and temperature. For mass diffusion in laminar flows, Fluent uses the Fick's law and the diffusion flux can be written as (Eq. 3):

$$\vec{Ji} = -\rho D_{i,m}\nabla Y_i + D_{T,i}\frac{\nabla T}{T} \quad [\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}] \qquad (3)$$

For mass diffusion in turbulent flows, the formula is of the following form (Eq. 4):

$$\vec{Ji} = -\left(\rho D_{i,m} + \frac{\mu_t}{Sc_t}\right)\nabla Y_i - D_{T,i}\frac{\nabla T}{T} \quad [\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}] \qquad (4)$$

where $D_{i,m}$ [m^2/s] is the mass diffusion coefficient for species *i*, D_T is the thermal diffusion coefficient [m^2/s], Sc_t is the turbulent Schmidt number (unitless) which is 0.7 as default and μ_t is the turbulent viscosity [m^2/s].

The turbulent diffusion generally overwhelms laminar diffusion and the specification of detailed laminar diffusion properties in turbulent flows is generally not necessary.

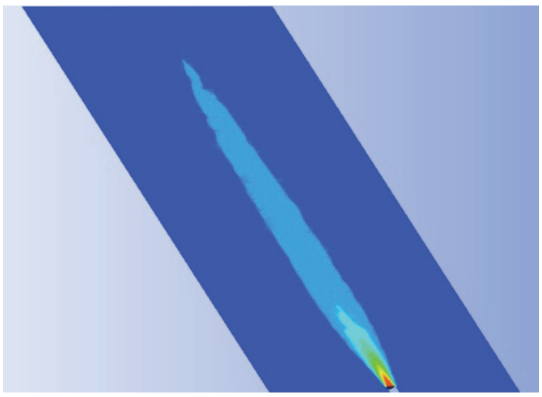

Fig. 7. Gas leak simulation performed in previous research works

Fig. 7 presents the situation of a jet release (flammable gas cloud formation) in case of a leak of methane having a surface of 1 mm^2, for open-air conditions, with a co-flow of 0.1 m/s.

The reaction rates which appear as source terms in Eq. (2) are computed in ANSYS Fluent, for turbulent flows, by one of three models: i) Laminar finite-rate model: The effects of turbulent fluctuations are ignored, and reaction rates are determined by Arrhenius kinetic expressions; ii) Eddy-dissipation model: Reaction rates are assumed to be controlled by the turbulence, so expensive Arrhenius chemical kinetic calculations can be avoided. The model is computationally cheap, but, for realistic results, only one or two step heat-release mechanisms should be used; iii) Eddy-dissipation-concept (EDC) model: Detailed Arrhenius chemical kinetics can be incorporated in turbulent flames. Note that detailed chemical kinetic calculations are computationally expensive.

The generalized finite-rate formulation is suitable for a wide range of applications including laminar or turbulent reaction systems, and combustion systems with premixed, non-premixed, or partially-premixed flames. Fig. 8 is the representation of the flame front development after an air-methane mixture explosion within a confined space, on its' path being figured obstacles in order to visualize their influence on the flame front and pressure wave propagation.

3.1.2. Numerical model validation

Due to the complexity of CFD codes and due to their continuously expanding range of possible applications, validation and verification are on-going activities. Prior to the release of a code, there should be carried out some basic verification and there should be performed basic validation studies on classes of flow characteristics before using the code for similar flows. However, verification and validation should continue as the code continues to develop.

The verification and validation of computational simulations carried out based on physical experiments will be performed by a comparative analysis of virtual results with the experimental ones. Moreover, even if a high similitude results after the analysis, the dependence of the solution on the resolution of the mesh will be tested.

Overcoming this stage for validating the mathematical model opens up the road to the main goal of the project: implementing the mathematical model on a spatial model at real scale, of a confined industrial area with explosion hazard. A complex analysis results from complex cases; therefore, for building up pressure and temperature diagrams from which to explicitly result the extent of hazardous area depending on the supportability level of the human body are required the results of simulations performed on geometries of various complexity.

As a consequence, the final result of will consist in a set of diagrams representing the hazardous area extent in case of explosions of flammable atmospheres generated by accidental gas leaks in confined spaces.

3.2. Experimental stand setup

According to the conditions which have to be fulfilled by domain for analyzing the flammable gas leaks the technical drawings for the experimental stand's sub-assemblies, as set out below, have been executed.

The explosion chamber shown schematically in Fig. 9 is a rectangular parallelepiped, with 20 mm thick transparent PMMA polymethacrylate walls, a material 30 times more durable than glass, having a volume of 60.3 liters (300 x 300 x 670 mm). The upper part of the explosion chamber shown in Fig. 10 is detachable to allow easy change of the physical conditions inside the confined space. The upper part of the explosion chamber is equipped with gaskets, hinges and butterfly nuts to ensure the tightness of the analysis domain. Also, an explosion overpressure discharger is located on the upper wall, as shown in Fig. 11.

A stand suitable for the dimensions of the explosion chamber was constructed to allow the placement and facilitate the curving of a conventional mirror in order to obtain the Schlieren effect. This is part of the experimental stand for the simulation of explosions caused by gas leaks in confined spaces, the experimental model being shown in Fig. 12.

3.3. Physical experiments, computational simulations and results

Physical experiments aimed at recording the phenomenon through Schlieren techniques were carried out on the stand designed for investigating the behavior of the flame front in case of explosions due to accidental gas leaks in confined spaces. The video materials obtained are post-processed for the purpose of visualizing as clear as possible the explosion process. By applying the Schlieren viewing technique in case of controlled explosions generated on specially designed stands, in the study of this phenomenology can be obtained remarkable results.

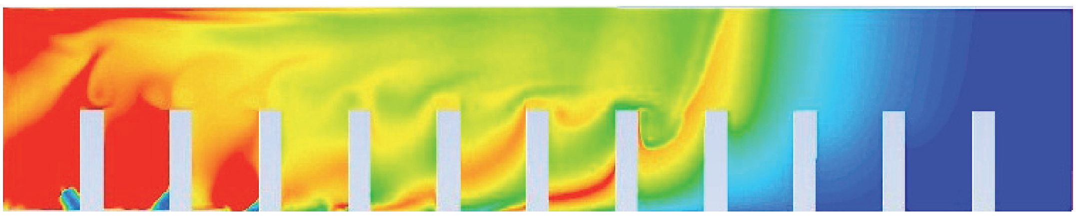

Fig. 8. Example of a computational simulation of air-methane explosion in a rectangular tube with obstacles, performed at INCD INSEMEX Petrosani

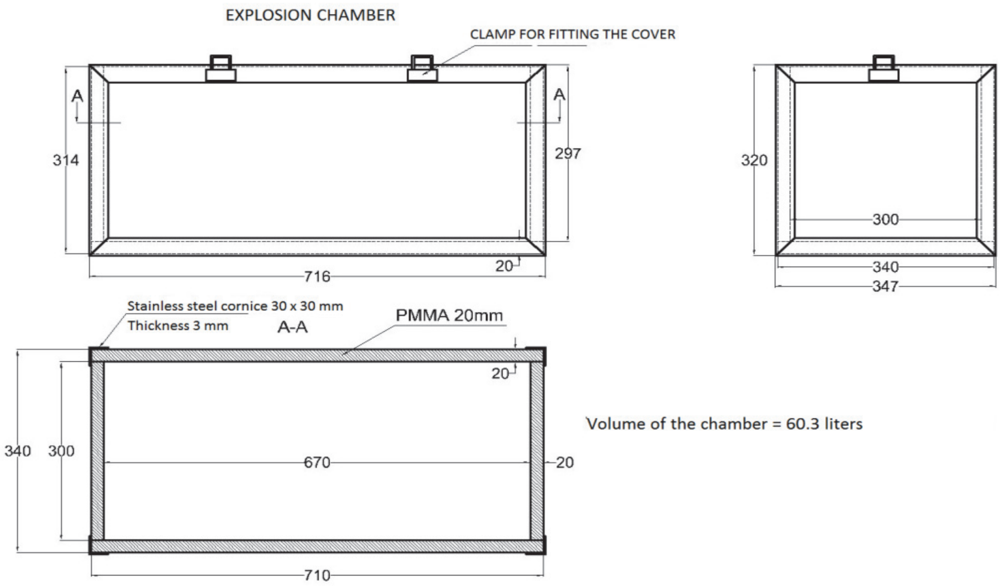

Fig. 9. Execution drawing of the explosion chamber

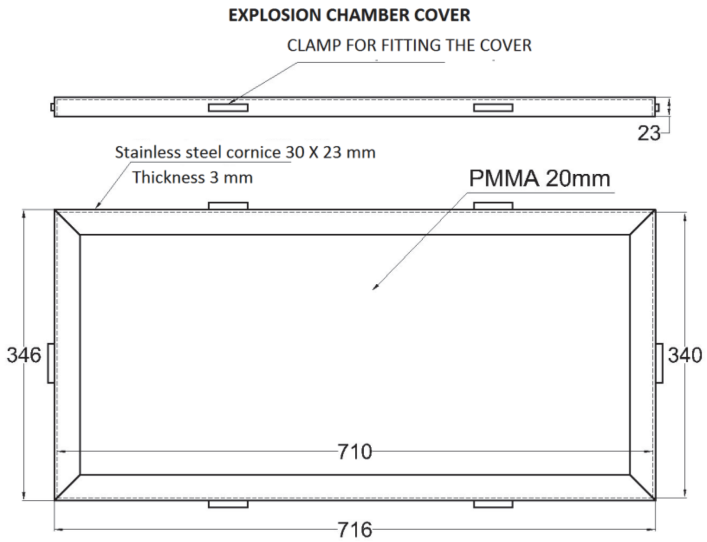

Fig. 10. Execution drawing of the detachable upper part

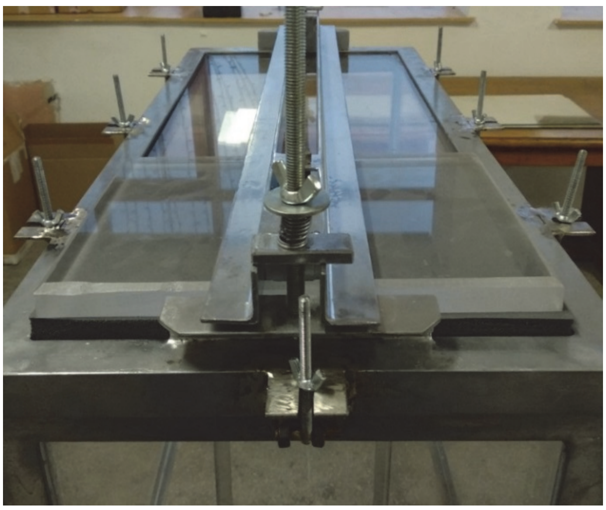

Fig. 11. The upper part of the experimental model for the analysis of gas leaks, fitted with an explosion pressure discharge device

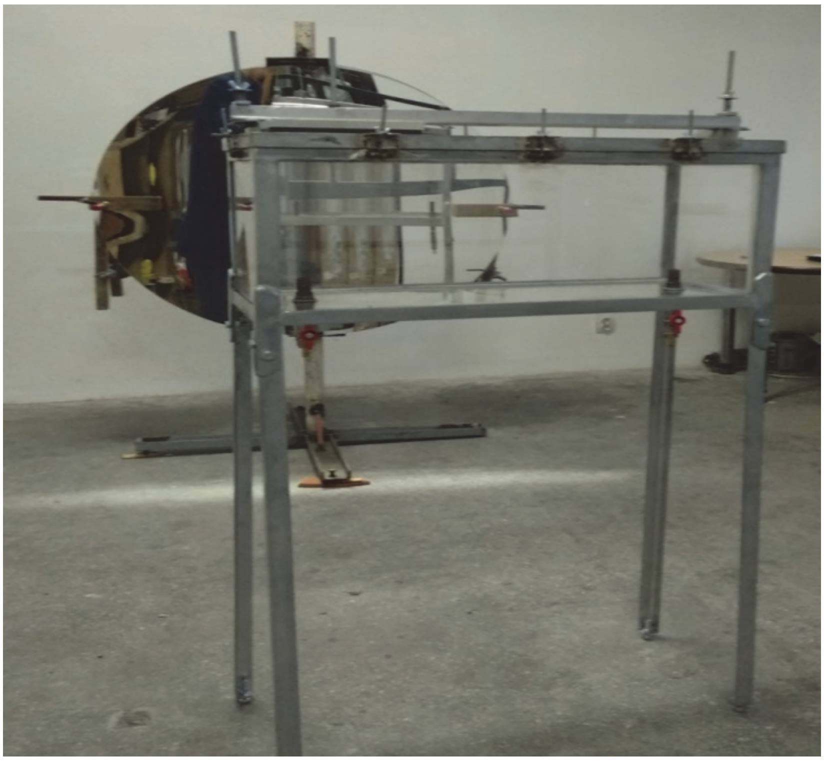

Fig. 12. Experimental model for analyzing gas leaks in confined spaces

At the same time, research equipment required is limited to the size of the laboratory, which means extremely low costs compared to the experiments carried out in large tubes where the explosion development visualization is almost impossible, monitoring being carried out only by pressure and / or light sensors. This effect is based on the existence of concentration gradients of mass particles, which causes the light beam propagation direction to change. In other words, the overall effect is more obvious as the density difference is more pronounced, being viewed as a shadow at the boundary between different values. On the background of the obtained images, important data were collected on the propagation of the flame front and the pressure wave inside the confined space. The results obtained from the physical experiments consist of data sets which are further used within the computational simulations.

For computational simulation purposes, the explosion chamber was transposed into the virtual space, with the initial setting of the field of analysis using input data identical to those used in the physical experiments on the formation, ignition and burning of air-gas atmospheres within the confined space. In this regard, for performing the computational simulation which to match the physical experiments carried out on the experimental stand, the virtual geometry of the explosion chamber was developed, considering the same dimensional values as those of the real model, consisting of a rectangular parallelepiped with the dimensions 300 x 300 x 670 mm (V = 60.3 litters). The upper part of the parallelepiped is provided with an orifice that has been transposed into the virtual model of the explosion chamber, being set as a movable wall which has its' own mass, thus reproducing the real model of the explosion pressure discharge device. In addition to the models used for defining the explosion of the fuel gas-air mixture within the rectangular parallelepiped, the dynamic mesh model was the main model used for defining the motion of the mobile border. Also, User Defined Function (UDFs) specific to dynamic mesh networks have been used in order to imprint the movement of the mobile border. In this sense it was possible to open the mobile border. The UDFs written in C programming language determine mathematically how the different areas of a mesh are deformed by translation / rotation and their dependence on certain parameters (e.g. pressure). UDFs are implemented within the Fluent Macros application. Using the DEFINE_CG_MOTION macro, for the present case, we could define the movement of the mobile border weight center (the physical pressure discharge device in case of physical experiments) based on the explosive pressure on the surface.

Computational simulations performed on the basis of user-defined functions have proven to be very close to physical experiments by achieving average flame front velocities between 8 and 8.6 m / s. Also, the behaviours of the flame front and of pressure wave were very similar in computerized simulations to those recorded in physical experiments. Figure 13 shows the behaviour of the flame front in the simulation of an explosion in the experimental chamber.

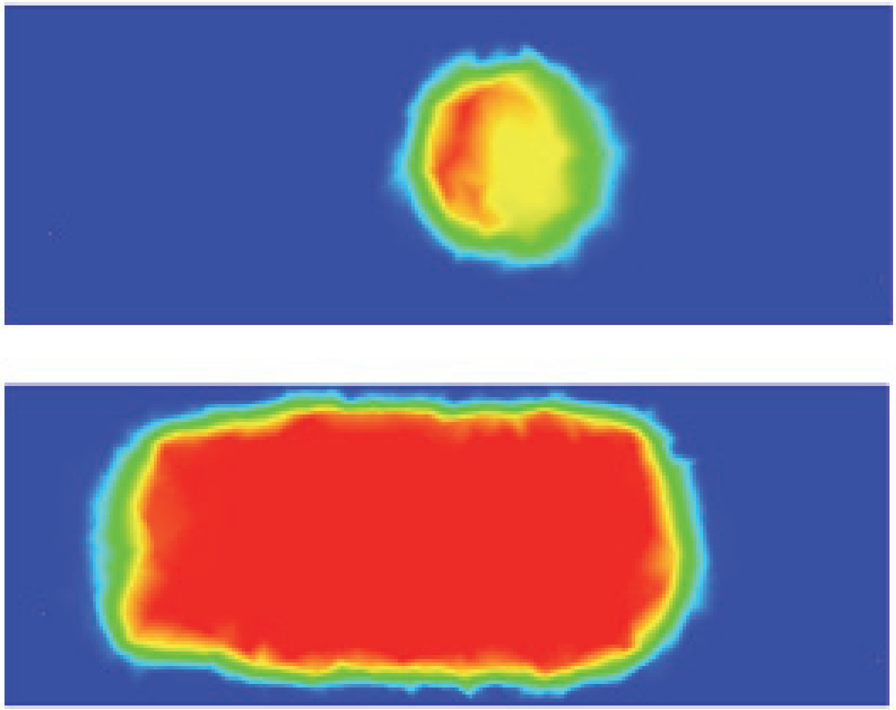

Fig. 13. Behaviour of the flame front at the beginning of the explosion process and in the explosion development phase

In both cases (the physical and computer simulation experiments), once with the increase of the pressure inside the explosion chamber, the pressure discharge provided at the top of the mobile border was pushed by the explosion pressure generated within the analysis domain, creating a free space where overpressure could be released. This results in a good correlation of the results obtained from the physical experiments and those obtained by performing virtual simulations, thus proving the validity of the computational simulations.

4. Conclusions

The research carried out for developing the novel computational tool for assessing the hazardous area extent in case of gas leak explosions in confined spaces relies on the following actions performed:

- Testing, selecting and calibrating mathematical models which are proper for simulating gas leaks, respectively explosions of flammable atmospheres in confined spaces.
- Validation of computational simulations, performed based on a comparative analysis of virtual results with the real ones.

The concept of the computational tool developed is based on the authors' previous results in experimental research on explosion-type phenomena and computer modeling and simulation of flammable gas dispersion and explosions of air-methane mixtures, placing the model at the beginning of the study on the Technological Readiness Level - TRL 2. The initial concept was developed, experimented in laboratory conditions and validated by comparison with the results of the experiments, and it can be said that the proposed model has reached the Technological Readiness Level TRL 4.

The significant result of the study is represented by the development of a numerical model that can be used as a reference and which is capable of faithfully reproducing explosions caused by accidental leaks of flammable gases in confined spaces, being useful in assessing the extent of the hazardous area generated by such events.

In the national and international context on explosion protection and of the new challenges in the field of occupational safety and health, it can be said that the study is of high importance, the demanding activities in this field being indispensable, even vital, for the economic operators in the industries with danger of explosive atmospheres, and also for the society. The numerical model can be used as a reference for subsequent design or analytical developments in confined industrial areas with explosion hazard.

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