

Computational Study of Scenarios Regarding Explosion Risk Mitigation

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Abstract. Exploration in order to discover new deposits of natural gas, upgrading techniques to exploit these resources and new ways to convert the heat capacity of these gases into industrial usable energy is the research areas of great interest around the globe. But all activities involving the handling of natural gas (exploitation, transport, combustion) are subjected to the same type of risk: the risk to explosion. Experiments carried out physical scenarios to determine ways to reduce this risk can be extremely costly, requiring suitable premises, equipment and apparatus, manpower, time and, not least, presenting the risk of personnel injury. Taking in account the above mentioned, the present paper deals with the possibility of studying the scenarios of gas explosion type events in virtual domain, exemplifying by performing a computer simulation of a stoichiometric air - methane explosion (methane is the main component of natural gas). The advantages of computer-assisted imply are the possibility of using complex virtual geometries of any form as the area of deployment phenomenon, the use of the same geometry for an infinite number of settings of initial parameters as input, total elimination the risk of personnel injury, decrease the execution time etc. Although computer simulations are hardware resources consuming and require specialized personnel to use the CFD (Computational Fluid Dynamics) techniques, the costs and risks associated with these methods are greatly diminished, presenting, in the same time, a major benefit in terms of execution time.

1. Introduction

Generally, all geological seams contain certain amounts of gases. By mining activities, some of these gases may be released in concentrations too low to take into account. The flammability properties of methane-air mixtures were frequently measured and summarized in publications, as methane is the main constituent of natural gas, mine gas or biogas [1]. Furthermore, the methane released from coal beds, together with minor amounts of hydrocarbons, carbon dioxide, nitrogen, oxygen, hydrogen and helium, is the main component of fire damp in a coal mine [2].

Because of the low level of sulphur oxides, hydrocarbons and carbon monoxides released when combusted, methane gas is viewed as a fuel with many environmental advantages [3]. But, with the advantages that this fuel gas brings, the risk of formation of explosive air-methane or oxygen-methane atmospheres occurs. Whatever the area where methane is present, uncontrolled bursts of this gas mixed with oxygen or air are totally undesirable events. Extreme events, which were considered improbable in the past, are now considered to be credible events, with a finite probability of occurrence [4].



Therefore, there where the possibility of forming these explosive atmospheres exists, explosion risk assessment is required by developing scenarios that consider the existence, in the same location and at the same time, the source of ignition, the combustible gas and the oxygen. Based on the ignition location of explosive mixture, the risk assessment must include the extension of dangerous area for the worst case: oxygen-methane stoichiometric reactions. This prediction is difficult, especially where space is occupied by technological equipment that impedes or makes impossible to predict the behaviour of the shock wave or of the flame front. If in case of simple geometries, it is possible to make some physical explosions experiments, in case of complex geometries or considerably extended surfaces these experiments cannot be performed due to the costs they imply. In this regard, CFD techniques can be very useful tools for risk assessors.

2. Domain setup and computational simulations

To emphasize by example those written above, a work hall was built roughly in virtual, in which they were arranged 3 boilers for steam generation (eg. for a power plant), as shown in Figure 1. The work hall by size of 50 x 30 x 10 meters has one access door on each short side. Through the first door enters an air flow rate of 0.01 kg/s, and the second door has been set as a free surface.

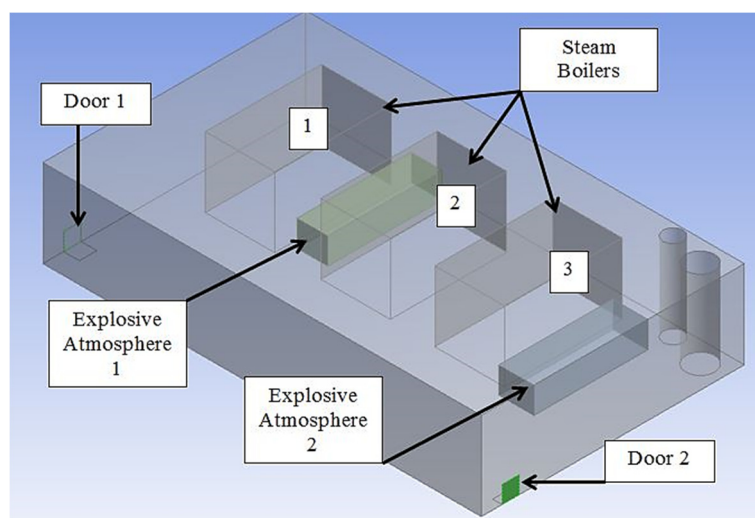


Figure 1. Virtual geometry of the work wall

Considering methane as the fuel used to produce the steam, there were simulated two scenarios for the explosion of an air-gas mixture formed by a leakage inside the hall. The first scenario involves the formation and initiation the explosive mixture in front of the boiler no. 1, and the second scenario examines the case of the ignition of the same explosive atmosphere in front of the boiler no 2. For each scenario were monitored the pressures acting on the doors and was observed the behaviour of the flame front.

2.1. Scenario 1

In front of the boiler no. 1 was set an explosive atmosphere consisting of air and methane at stoichiometric concentration in a volume of 13 x 3.5 x 3 meters, mixture assumed to be the result of a leakage in the supply line. The remaining volume of the hall was set to air features and the initiation of the explosive mixture was carried out by a spark at 1 meter from the floor. The temperature was observed, as colour contours of a dynamic scale, on a vertical section through the location of the spark (Figure 2) and on the horizontal section at 1 meter from the floor. (Figure 3). Initial time t_0 is the time of the mixture ignition.

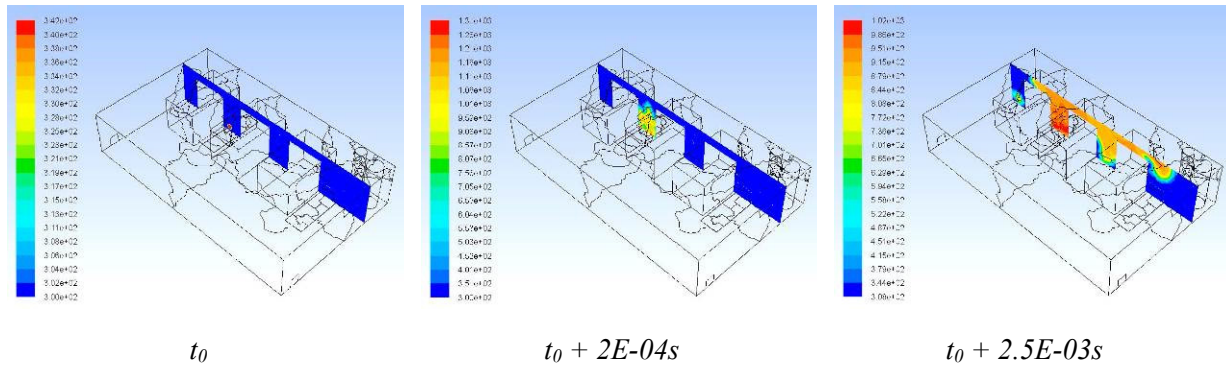


Figure 2. Temperatures on vertical section at different times

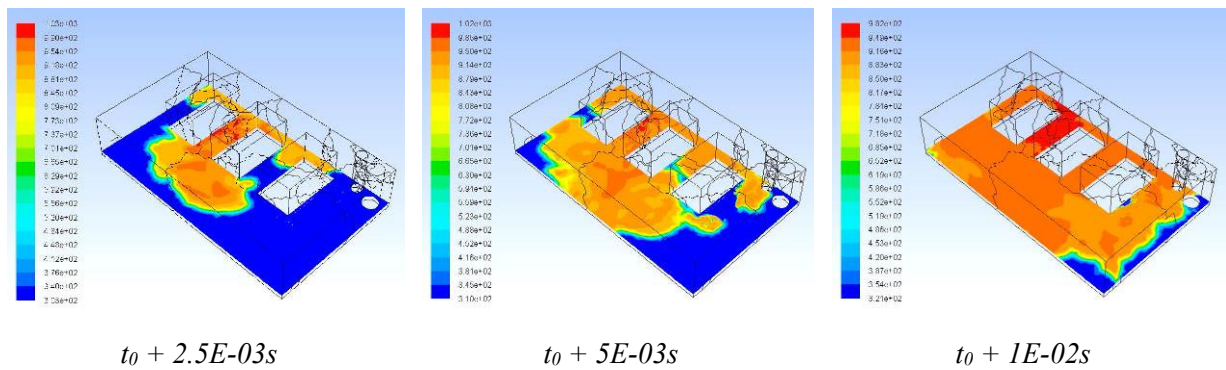


Figure 3. Temperatures on horizontal section at different times

The pressures were monitored on the surfaces of the access doors and were observed, as colour contours of a dynamic scale, on the same section at 1 meter from the floor (Figure 4).

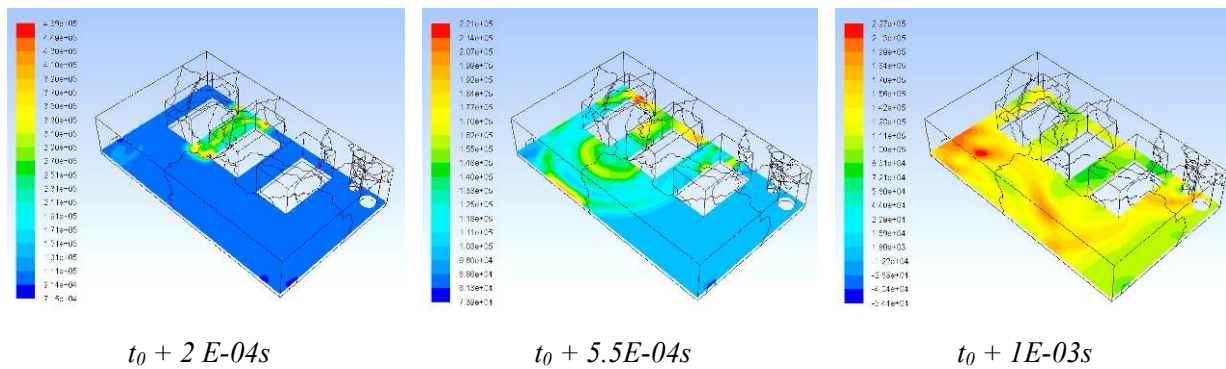


Figure 4. Pressures on horizontal section at different times

2.1. Scenario 2

Keeping the same settings of methane-air mixture and the same boundary conditions for access doors for the second scenario of an explosion inside the work wall, the accumulation of gas and the formation of the explosive atmosphere in front of the boiler no. 3 was considered. The location of the spark was at 1 meter from the floor. As in the first scenario, the temperature was observed, as colour contours of a dynamic scale, on a vertical section through the location of the spark (Figure 5) and on the horizontal section at 1 meter from the floor and (Figure 6).

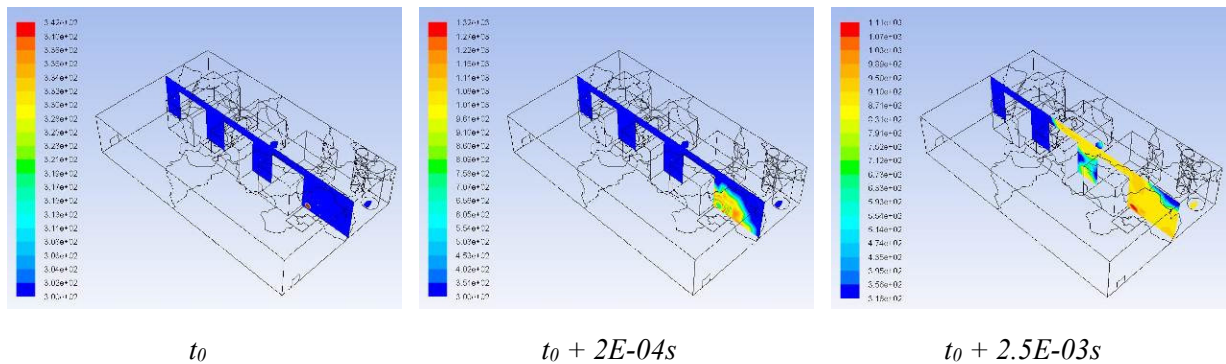


Figure 5. Temperatures on vertical section at different times

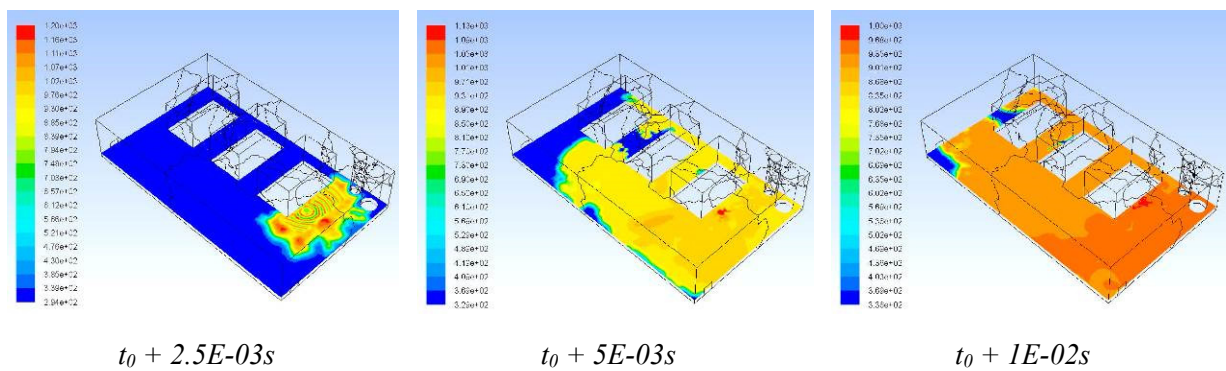


Figure 6. Temperatures on horizontal section at different times

The pressures were monitored on the surfaces of the access doors and were observed, as colour contours of a dynamic scale, on the same section at 1 meter from the floor (Figure 7).

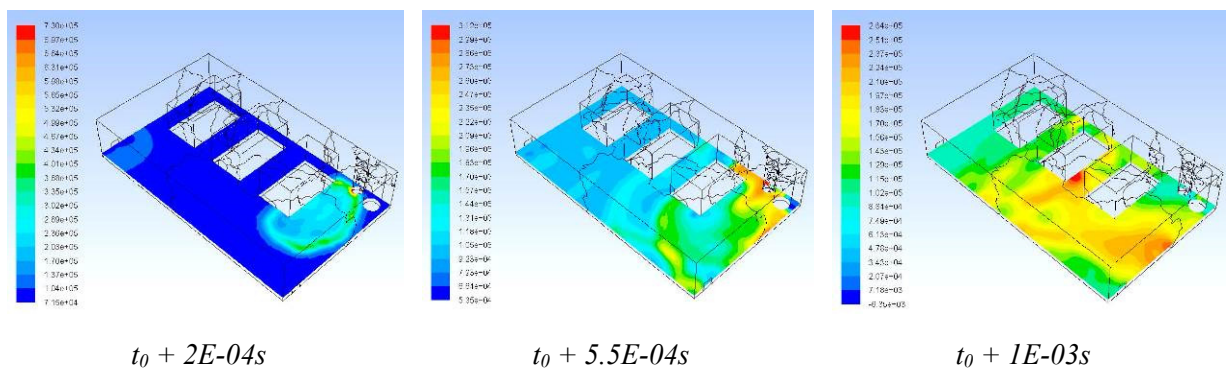


Figure 7. Pressures on horizontal section at different times

All the captures were made at the same times as in first scenario.

3. Results and discussions

Computational simulations presented in this paper were performed in FLUENT application belonging to ANSYS Multiphysics package. This package has all the necessary tools to mathematical model the fluid flow, from building the virtual geometry and meshing it in desired method, to post processing the results of the calculations.

The model used to perform the simulations was a transient, pressure-based one, applying the Large Eddy Simulation method (LES). To avoid reaching high temperatures of over 5000 K using the default settings of the application, for the specific heat of air-methane mixture has implemented a polynomial

function of degree 4. The coefficients of this function were determined so that, in the detonation simulation of an air-methane stoichiometric mixture, the flame temperature to be close to the value of 2223 K from literature [5]. The polynomial function for specific heat at constant pressure, c_p , is described as:

$$c_p = a_0 + a_1T + a_2T^2 + a_3T^3 + a_4T^4 \quad (1)$$

where T is the temperature and the coefficients used are in the following values (Table 1):

Table 1. α - coefficients

a_0	a_1	a_2	a_3	a_4
321.3016	6.55905	9.22653E-06	-3.43396E-09	4.74731E-13

The reactions used for methane oxidation was 2 step Westbrook and Dryer mechanism. Since in both cases the volume of the explosive atmosphere has not been separated from the volume of the boiler house by any wall, the methane tended to dissipate to the front of the flame, burning at lower concentrations, up to its consumption. Thus, the maximum temperature achieved in the combustion process was up to 1400 K (Figure 8).

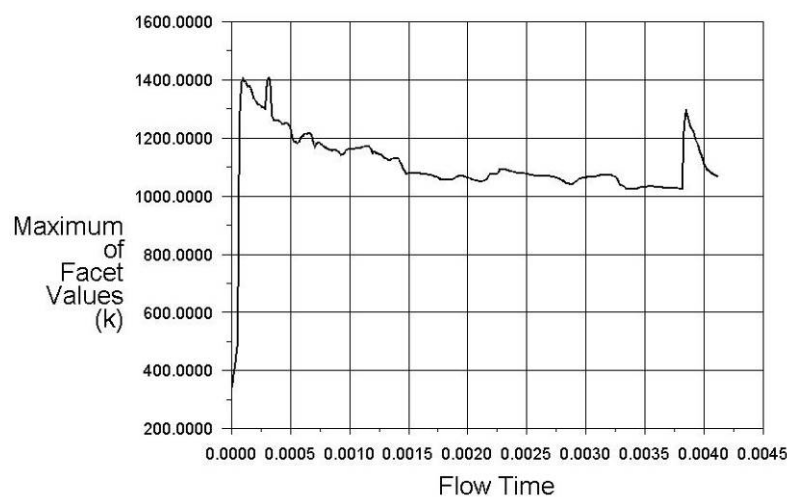


Figure 8. Maximum facet temperature on vertical section

Also, in the temperatures graph it can be seen an ignition of an air-methane explosive hose at about 0.0038 seconds from mixture ignition. The monitored pressures on surfaces of access doors, for both scenarios, are shown in Figure 9 and Figure 10. For the first scenario, the pressure reached on Door 2 is about 350 000 Pa lower than that measured on Door 1. But the pressures on both doors from second scenario are about the same values as the pressure on Door 1 – first scenario.

4. Conclusions

First of all, this work wants to be an example of the use of CFD techniques in explosion risk assessment. In this example, once again it is proven the explosion hazard around the work hall in case of a leakage of the combustion gases. But, with the use of these CFD tools, multi-criteria decision problems can be resolved much easier. Through further analysis, the risk of explosion can be minimized by placing pressure release devices in locations where computational simulations show

high pressures. However, analysis carried out by these techniques must be done with great responsibility, because the introduction of erroneous input data and improper intervention of the analyst in the calculating process can lead to dangerous results to be used in practice.

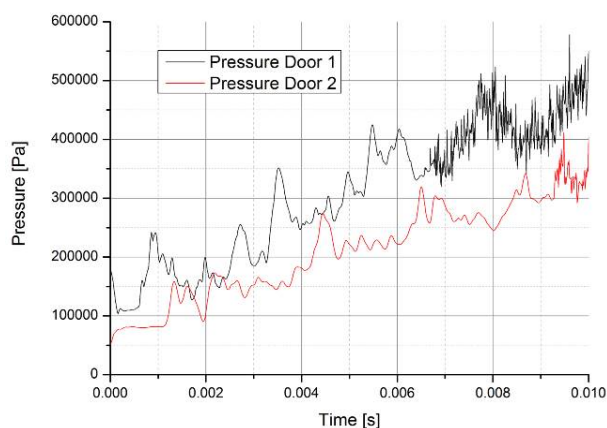


Figure 9. Values of pressure on doors surfaces for the first scenario

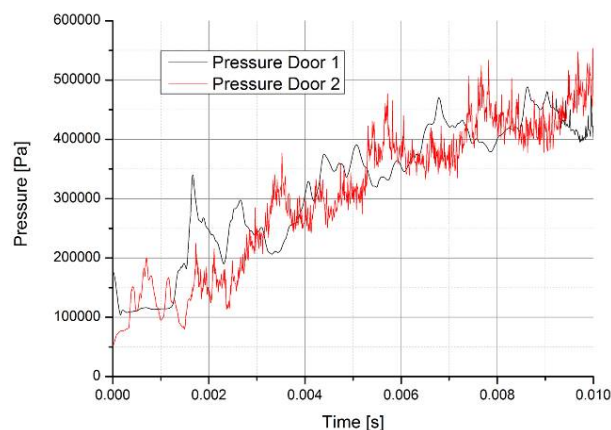


Figure 10. Values of pressure on doors surfaces for the second scenario

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