Release of overpressures in computational simulations of air-methane explosions

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Abstract. Research in the field of gas explosions has had and continues to have, as its main support, physical experiments performed on various scale models, the construction of real size models are often large consuming materials, time and labor. The rapid development of computing techniques has allowed among other things, the transfer of gas explosions research in the virtual space, for the validation of computational simulations of this type being still considered physical experiments and specialty literature. Within NIRD INSEMEX Petrosani, being an accredited institute in the elaboration of technical reports for gas explosion type events, the phenomenon of rapid combustion virtualization increased in time and as a result, computational simulations becoming an efficient tools in explaining the mechanisms of explosion production. Nevertheless, one of the problems raised by this virtualization process is the limitation of performing computational simulations in closed or partially closed spaces, initial conditions imposed, without the possibility of dynamic modification of these conditions according to the development of overpressures generated by the virtual explosion. This paper presents a computational experiment in which it was possible to transform the boundary conditions at predefined pressure thresholds, from rigid surfaces into surfaces capable of releasing the overpressures developed in closed / partially closed spaces, putting the results of this kind of simulations in line with real dynamic effects of gas explosion events.

1 Introduction

In order to obtain results as close as possible to reality, new ways of staging the computational simulation were tested. It is well known that the explosion overpressures are the main culprits of the devastating dynamic effects in the case of gas explosion events. In closed spaces, these overpressures are carried out with increased aggression [1, 2]. However, where there are low-strength surfaces (eg glazed surfaces, wooden doors, etc.), overpressures are partly released when they break, leading to a significant reduction in the dynamic effects of the affected space. This scenario, at least in the case of using the ANSYS Multiphysics platform, is impossible to implement in computational simulations without the contribution of user-defined functions. (UDF – User Defined Functions) written

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in the C language and, moreover, without instruction files written in SCHEME code that accompany the UDFs.

In this paper it has been tested such a scenario, in a rectangular tube with obstacles being made a virtual explosion of a stoichiometric mixture air - methane gas. Initially being a closed space, when exceeding a pressure threshold, the transformation of the end surface opposite to the area of initiation of the explosive atmosphere, from a wall type surface (as a input parameter: WALL) to an open surface (as a output parameter: Pressure Outlet) by means of UDFs and codes Schemes mentioned above. [3].

2. Setting the computational domain

All the virtual activities, including geometry construction, meshing, setting the boundary conditions, solving and post-processing were performed in ANSYS Multiphysics package. ANSYS Fluent was used to define the domain properties and calculate the results [4]. The Fluent application is based on finite elements or finite volume methods and can perform 2D and 3D simulations of various types of problems including multi-component and multi-phase flows, compressible flows, flows with heat transfer, cavitation and other phenomena.

2.1 Geometry and meshing

The virtual geometry consists of a rectangular tube of dimensions1000x100x100 mm, provided with 4 obstacles of increasing height from the area of initiation of the explosion to the right end of the tube (colored in green in fig.1).

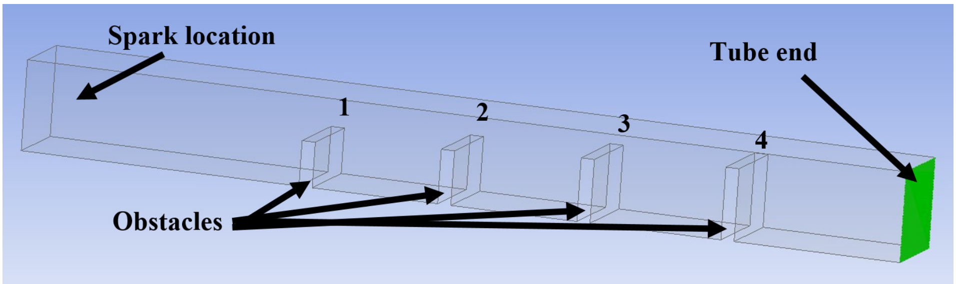


Fig. 1. Virtual geometry.

The geometry thus constructed was discretized into 26.496 finite volumes and 31.620 nodes (fig. 2.), mesh supported by the solver for processing fluid media.

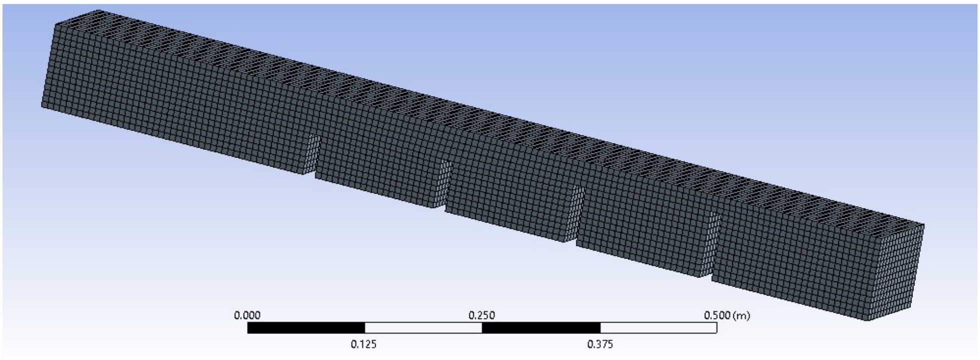


Fig. 2. Discretized geometry.

In this phase they were also set as (Named_Selections) the areas necessary for the transformation / taking over of the results from the following phases:

- The end of the tube: End_tube;
- End of the tube, from the spark location: First_tube.

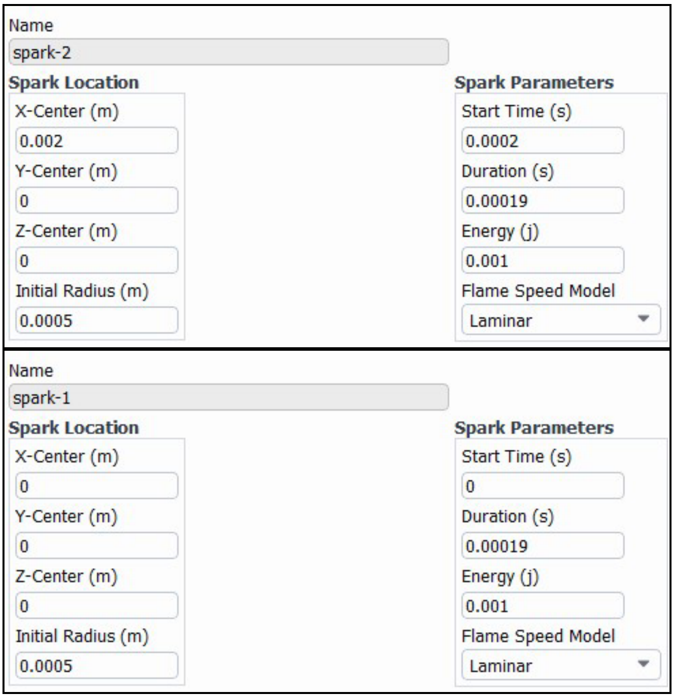
And the areas from the spark location of each obstacle, starting with obstacle 1:

- Obstacle_1;
- Obstacle_2;
- Obstacle_3;
- Obstacle_4.

2.2 Domain setup

The inner atmosphere of the tube was set at a concentration of 9.5% vol. CH_4 and at a temperature of 20°C.

As for the location of the spark, it has been set as moving over time, simulating the movement of a mechanical spark in the explosive atmosphere, with a speed of 10m/s This movement is achieved by setting 6 sparks that are activated / deactivated successively, following a trajectory from the first location towards the first obstacle, as shown in fig. 3, for the first two sparks. The sparks have an energy of 0.001 J and have a radius of 0.5 mm.



Name
spark-2

Spark Location
X-Center (m): 0.002
Y-Center (m): 0
Z-Center (m): 0
Initial Radius (m): 0.0005

Spark Parameters
Start Time (s): 0.0002
Duration (s): 0.00019
Energy (j): 0.001
Flame Speed Model: Laminar

Name
spark-1

Spark Location
X-Center (m): 0
Y-Center (m): 0
Z-Center (m): 0
Initial Radius (m): 0.0005

Spark Parameters
Start Time (s): 0
Duration (s): 0.00019
Energy (j): 0.001
Flame Speed Model: Laminar

Fig. 3. Series of two sparks out of a total of 6, simulating the movement of a mechanical spark.

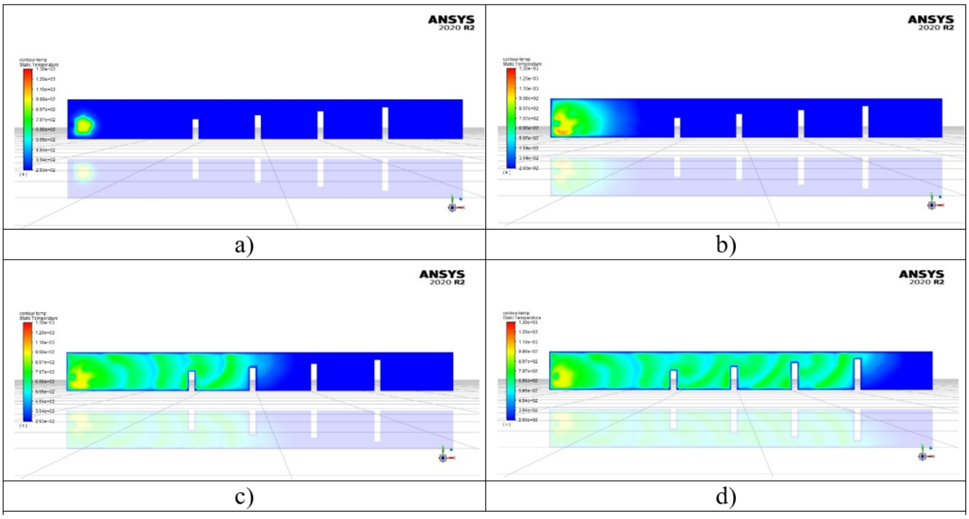
The end of the tube (to be transformed) was initially set as a wall surface at a temperature of 20°C.

A C code was written to transform the surface, based on the DEFINE ADJUST macro, dedicated to the ANSYS Fluent application solver, by which the threshold of 108325 Pa is set for opening the surface and have the role of setting the surface at the end of the tube as “Pressure outlet” to the signal received from the previous specified macro. Also, the instructions set an external pressure value of 101325 Pa and a temperature of 293 K - atmospheric pressure and temperature of 20^{o}C.

3. Computational simulations

In the following images are highlighted some moments from the development of the rapid combustion process of the explosive atmosphere air - methane gas inside the tube:

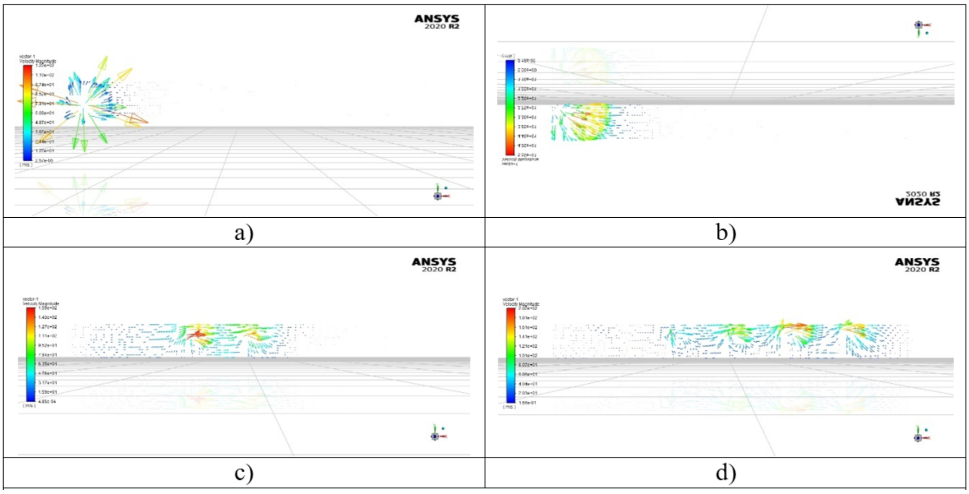
Color contours of temperatures:



a) b) c) d)

Fig. 4. Sequence of images with colour contours of temperatures.

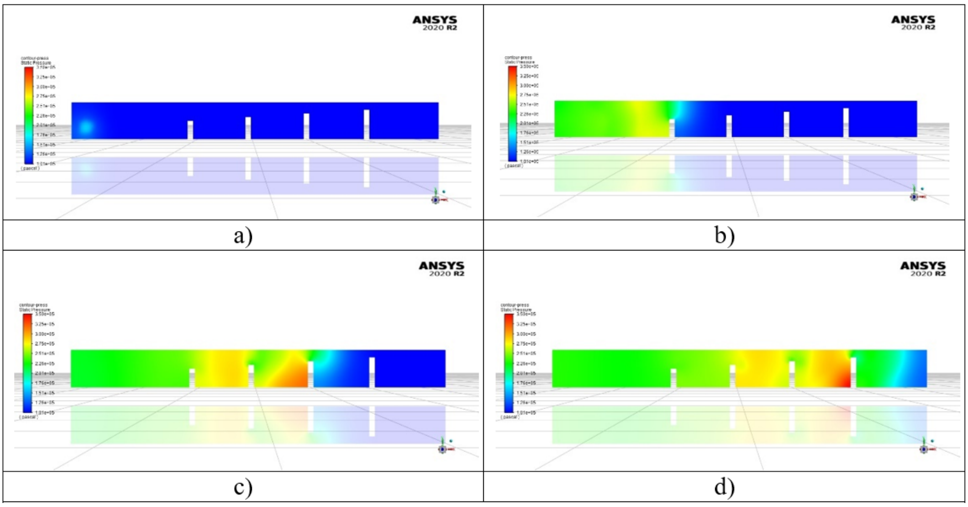
Vectors velocity:



a) b) c) d)

Fig. 5. Sequence of images with velocity vectors.

Color contours of pressures:



a) b)

c) d)

Fig. 6. Sequence of images with color contours of the pressures.

4. Results

As a result of the calculation process, the pressures on the surfaces (Named Selections) were registered in separate files defined in the preparation phases of the simulation. These data were imported into an Excel file and superimposed, resulting in pressure variations in fig. 7.

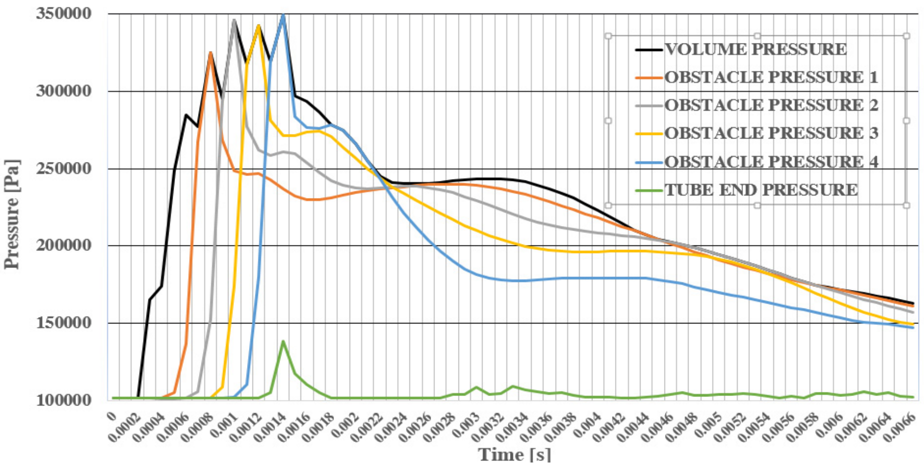
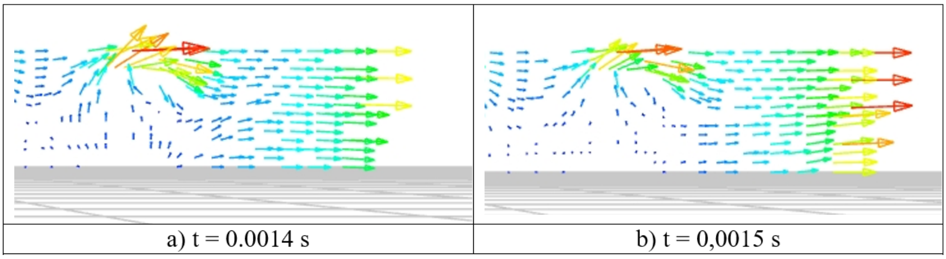


Fig. 7. Variations in pressure in volume and on surfaces in the analysed range.

Figure 8 shows images obtained at times t = 0.0014 and t = 0.0015 s, times during which the pressure threshold set by the UDF has been exceeded. Figure 8 b) shows velocity vectors higher than those in Figure 8 a), which means opening the end of the tube (transforming this surface from the Wall into a Pressure Outlet) and release of explosion pressures, [5, 6]. This fact is confirmed by the decrease of pressures from the entire volume of the rectangular tube starting with this moment and the tendency of the curves to the value of atmospheric pressure [7].



a) t = 0.0014 s

b) t = 0,0015 s

Fig. 8. Release the explosion overpressure when the set pressure threshold is exceeded.

5. Conclusions

In this paper was achieved a computational simulation through which the explosion process of an explosive mixture of air - methane gas was highlighted, from initiation to release of the explosion pressures.

The initiation of the explosive atmosphere was simulated by a mechanical spark, with movement in the explosive environment, this being able to constitute an efficient source of ignition.

The virtual explosion of the air-methane gas mixture took place inside a rectangular tube provided with obstacles of different sizes, provided with a low resistance area, which yielded to a pre-set pressure threshold releasing explosion overpressures, being simulated, the glazed surfaces of a real room. In this way, the results of future simulations performed on virtual scale models, in possible gas explosion scenarios, they can highlight more explicitly the mechanisms underlying this type of event.

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