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COMPUTATIONAL SIMULATION OF METHANE IGNITION IN ENCLOSED SPACES

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Abstract: *In the research on gas explosions, the emphasis has been and continues to be primarily on physical experiments conducted on various scaled-down models. Building models at actual size is often a resource-intensive task in terms of materials, time, and human resources. The rapid advancement of computational techniques has allowed, among other things, the transfer of gas explosion research into the virtual environment. For validating computerized simulations of this kind, physical experiments and specialized literature are still considered fundamental. However, one of the challenges posed by the virtualization process is the limitation of conducting simulations in fully or partially enclosed spaces, under initially imposed conditions, without the possibility of dynamically modifying these conditions based on the development of overpressures generated by the virtual explosion. This paper details a computerized experiment where the boundary conditions were successfully transformed into predefined pressure threshold surfaces, transitioning from rigid surfaces to surfaces capable of releasing the overpressures developed in fully or partially enclosed spaces. This approach aligns the results of these simulations with the real dynamic effects of gas explosion events***.**
Keywords: *accidental leakage, explosion, methane gas, methane ignition, CFD, Ansys*

1. Introduction

Computerized modelling of explosion phenomena in enclosed spaces involves simulating the movement of zones based on the pressures generated by the event [1], [2], [3], deformation through translation and/or rotation of these zones, or even transforming their conditions from wall-type boundaries to open boundaries to release explosion pressures.

In this context, the present paper aims to analyse virtual modelling methods of explosions in interconnected enclosed spaces using existing models within the ANSYS Fluent application. These models allow for defining the translation/rotation movements of discretization networks, including the sliding mesh model and the dynamic mesh model [4], [5].

The sliding mesh model allows for setting up problems where separate zones of the studied domain have relative movements to each other. The relative movement of static and moving components (e.g., components of a rotating machine) leads to transient interactions [6]. Often, the transient solution sought in a simulation using the sliding mesh discretization method is periodic over time. Therefore, the transient solution repeats, with a period dependent on the speeds of the moving domains.

The dynamic mesh model allows for the movement of the boundary of one cell zone relative to other boundaries of the zone, for appropriate adjustment of the mesh [7], [8]. Boundaries can have rigid rotation or translation movements dependent on each other, and/or deformation movements.

The decision to use sliding versus dynamic mesh discretization [9] considers the following:

- Most problems can be solved using both methods;
- In cases where the problem does not involve the deformation of the discretization mesh, the sliding method is recommended as it is simpler and more efficient;

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- The dynamic mesh discretization method should be used in the case of deformations or when the movement of the mesh is a function of the solution (for example, when invoking the Six Degree of Freedom solver – six degrees of freedom).

With the introduction of computerized simulations in various industries or even for household demonstrations, the need arose to verify and validate the results of these tools by comparing the obtained data with those from corresponding physical experiments [10], [11].

The verification of results can consist of several stages:

- Verifying the soundness in choosing the mathematical model;
- Checking the solution's conformity with boundary conditions imposed by the mathematical model;
- Verifying the correct correspondence between the CFD solution and the principles of the mathematical model (mass, momentum, energy conservation);
- Verifying the acceptability of linearization errors in processing governing equations;
- Verifying the acceptability of discretization errors by running the simulation - using the same input data - on a refined discretization network [12] for comparing result sets;
- Verifying the conformity of the CFD solution with the analytic solution in the region of full flow development.

The validation of results involves the comparative process of data and the acceptance or rejection of a certain level of deviation from results obtained from experiments.

The verification and validation of computerized simulations, in the simplest and most accurate manner, are achieved through a comparative analysis of results from physical experiments with those obtained in the virtual environment, considering the same geometric conditions and fluid properties in both domains (physical and virtual).

2. Computational Fluid Dynamics

Numerical Fluid Mechanics (NFM), also referred to as Computerized Fluid Mechanics, emerges from the branch of Fluid Mechanics. It utilizes algorithms, numerical methods, and computers to model and solve problems involving fluid flows.

Numerical simulation methods were initially designed for solving linearized equations of the potential field. In the 1930s, two-dimensional methods were developed to address flows around aerodynamic profiles. The first scientific communication regarding a method to solve linearized potential field equations was published in 1967 by John Hess and A.M.O. Smith from Douglas Aircraft. They discretized surfaces with panels and developed a class of algorithms called the panel method, applied to ship bodies and aircraft fuselages. The initial application of the panel method for lifting flows, Panel Code, was described in a 1968 scientific communication by Paul Rubbert and Gary Saaris from Boeing Aircraft. Subsequently, several programs based on the same method were developed by Lockheed, McDonnell Aircraft, NASA, and Analytical Methods [13].

In 1975, the FLO22 program was written for three-dimensional potential flows, leading to various applications, including Boeing's Tranair, still in use today. In 1985, Antony Jameson developed the three-dimensional AIRPLANE program using tetrahedral discretization. In the two-dimensional domain, Mark Drela and Michael Giles wrote the ISES Euler program in 1986 for designing aerodynamic profiles.

Programmers' ultimate goal was to model based on the Navier–Stokes equations. NASA developed the two-dimensional ARC2D program and the three-dimensional programs ARC3D, OVERFLOW, CFL3D, forming the basis for numerous commercial applications.

In the 1980s, solving fluid flow problems through CFD was confined to academic, post-doctoral, or post-university research, involving experts with many years of experience. The current availability of engineering workstations (computers), along with efficient solution algorithms and sophisticated pre- and post-production processing facilities, enables engineers and researchers to use commercial CFD codes in development and industrial design activities. Current market codes can be powerful, but their operation requires a high level of suitable expertise and the user's understanding of physical/chemical processes to obtain meaningful results in complex situations [14], [15].

Another aim of CFD development is to provide capabilities comparable to other Computer-Aided Engineering (CAE) tools, such as stress analysis codes. The main reason for CFD's delay was the immense complexity of basic behaviour, making it impossible to economically and sufficiently describe fluid flow. Affordable high-performance computing components and the introduction of intuitive interfaces have led to a recent surge in interest, and CFD is ready to enter the large industrial community in the 1990s.

vol. 30, issue 1 / 2024
pp. 58-67

Investment costs in CFD capabilities are not small, but total expenses are generally not as high as those for high-quality experimental facilities. Moreover, compared to the experimental approach to fluid system design [16], CFD has several unique advantages:

- Substantial reduction in time and costs for new projects;
- Ability to study systems where controlled experiments are difficult or impossible (e.g., very large, complex systems);
- Ability to study systems with hazardous conditions and beyond normal performance limits (e.g., studying risk factors and accident scenarios);
- Practically unlimited level of result details.

In addition to substantial investment, qualified personnel are needed to run the codes and communicate the results.

3. Computational Simulation with the use of User-Defined Functions

In order to obtain results as close to reality as possible, new methods of implementing computerized simulations have been explored. It is well known that the high pressures generated by explosions are the main causes of devastating dynamic effects in the case of gas explosion events [17]. In enclosed spaces, these high pressures manifest with increased aggressiveness. However, in areas where there are surfaces with low resistance (such as glass surfaces, wooden doors, etc.), a portion of the high pressures is released by breaking them, leading to a significant reduction in dynamic effects in the affected space. Implementing such a scenario, at least in computerized simulations using the ANSYS multiphysics platform, is challenging without the involvement of user-defined functions (UDF) written in the C language and, additionally, without instruction files written in the SCHEME code accompanying these UDFs [18].

In this paper, we tested such a scenario by simulating a virtual explosion of a stoichiometric mixture of air and methane in a rectangular tube with obstacles. Initially, within a confined space, we investigated the transformation of the surface opposite the initiation area of the explosive atmosphere, transitioning from a wall-type surface to an open surface (Pressure Outlet), using the aforementioned UDFs and Scheme codes.

3.1 Configuring the Geometric layout and mesh structure

This configuration involves the use of a rectangular tube with dimensions of 100x10x10 cm, where four obstacles have been integrated in ascending order of height. These obstacles extend from the explosion initiation zone towards the right end of the tube and are highlighted in green in Figure 1.

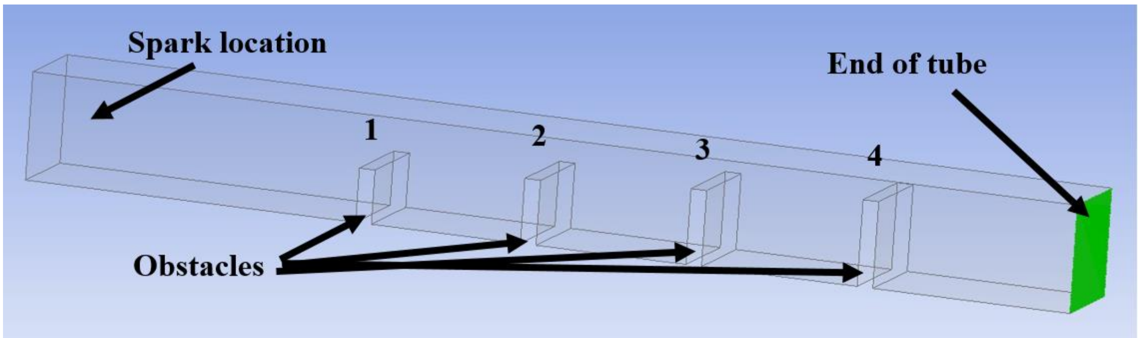


Fig.1. Virtual geometry of rectangular tube

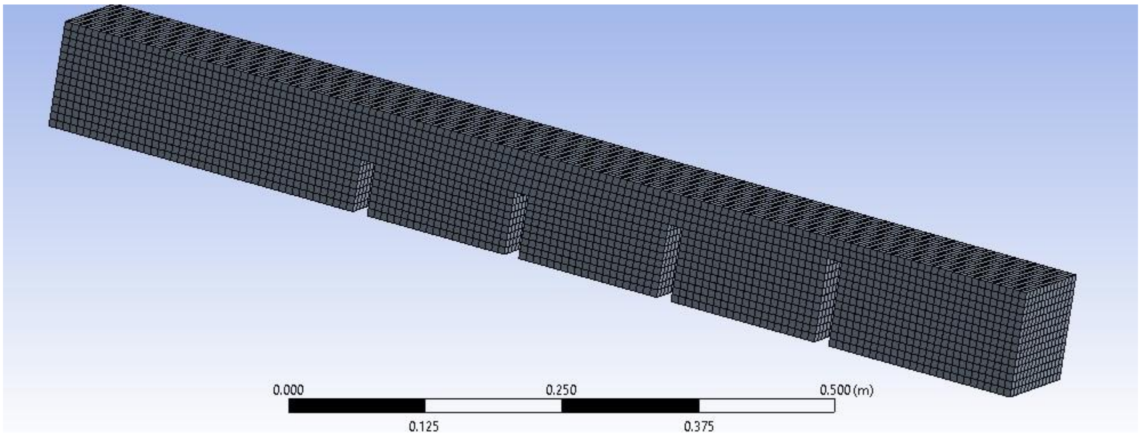


Fig.2. Discretized geometry

Revista Minelor – Mining Revue vol. 30, issue 1 / 2024
ISSN-L 1220-2053 / ISSN 2247-8590 pp. 58-67

The virtual geometry constructed in this manner has been intricately segmented into 26,496 finite volumes and 31,620 nodes, as depicted in Figure 2. This intricate mesh has been chosen in accordance with the requirements of the solver specialized in fluid medium processing.

Certain areas have been identified and marked as (Named_Selections), which are necessary for the transformation process. These zones can be selected to extract data or for post-processing of the results obtained in the virtual simulation. By establishing these named selections, it facilitates the management and efficient access to data, optimizing the workflow for future analyses. This practice is crucial for ensuring a coherent and precise analysis of the results.

- 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 no. 1:

- Obstacle no. 1;
- Obstacle no. 2;
- Obstacle no. 3;
- Obstacle no. 4.

3.2 Input parameters for domain setup

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

Regarding the spark's location, it has been configured to be in motion, simulating the movement of a mechanical spark in the explosive atmosphere, at a speed of 10 m/s. This movement is achieved by setting 6 sparks that are activated and deactivated successively, following a trajectory from the initial 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 a diameter of 0.5 mm.

This configuration allows for the simulation of spark movement in a flammable environment and is crucial for ignition and explosion propagation.

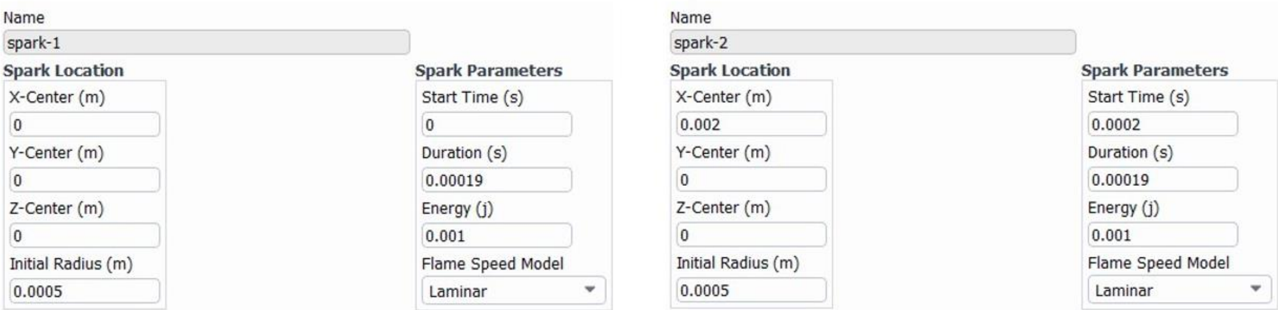


Fig. 3. Series of two sparks out of a total of 6, simulating the movement of a mechanical spark

The end of the tube, slated for transformation, was initially configured as a wall-type surface at a temperature of 20°C. To execute this transformation, a code was developed in the C language, based on the DEFINE ADJUST macro, specifically designed for the solver within the ANSYS Fluent application. Through this code, a threshold of 108,325 Pa was set for opening the surface:

```
#include "udf.h"
 #define FACE_ZONE_ID 6
DEFINE_ADJUST(door_break, d)
{
  int ID;
  face_t f;
  real maxPressure;
  int x;
    Thread* thread;
  /*Domain* d; */
  maxPressure = -9.99e30;
  x = 0;
 /* d = Get_Domain(1);  */
  thread = Lookup_Thread(d, FACE_ZONE_ID);
```

vol. 30, issue 1 / 2024
pp. 58-67

```
  begin_f_loop(f, thread)
  {
    if (F_P(f, thread) > maxPressure)
      maxPressure = F_P(f, thread);
  }
  end_f_loop(f, thread)
  /* In parallel, get the combined max pressure across all nodes: */
#if RP_NODE
  maxPressure = PRF_GRHIGH1(maxPressure);
  x = PRF_GRHIGH1 (x);
#endif
  /*Message0("\nMax Pressure = %f \n",maxPressure);*/
  if(maxPressure > 108325) {
     x = 1;
              }
  /* In parallel, send the combined max pressure to the host: */
   node_to_host_real_1(maxPressure);
   node_to_host_int_1(x);

  /* In parallel, only the host sets RP variables: */
#if !RP_NODE
              if(x > 0) {
    RP_Set_Integer("door_break/flag",1);
              }
  #endif
}
```

The SCHEME instructions are in the following format:

```
(rp-var-define 'door_break/flag 0 'integer 1)
(define (door)
(%rpgetvar 'door_break/flag)
(if (> (%rpgetvar 'door_break/flag) 0)
(begin
(ti-menu-load-string "define/boundary-conditions/zone-type 6 pressure-outlet")
(ti-menu-load-string "define/boundary-conditions pressure-outlet 6 yes no 101325 no 293")
)
 )
  )
```

and these instructions request configuring the surface at the end of the tube as a “Pressure outlet”. This indicates that for that surface, the pressure is known and considered to be an output value of the system. The signal necessary for this configuration is received from a previous macro, indicating that there is a preceding sequence of analysis providing these necessary pieces of information.

The instructions also set the values for the external pressure and temperature. The external pressure is set to 101,325 Pa, which corresponds to atmospheric pressure, and the external temperature is set to 293 K, equivalent to a temperature of 20°C. These values are essential for accurately modelling the environmental conditions and influence the behaviour of fluid flow. These instructions are crucial for establishing the necessary initial and boundary conditions to achieve a precise and relevant simulation of fluid behaviour. They ensure that the simulation is conducted in an appropriate environment and that the output conditions are suitable for subsequent analysis of the results.

3.3 Computational simulation

Following the virtual simulation of the rapid combustion process of the explosive mixture consisting of air and methane gas inside the tube equipped with obstacles, a series of data and information have been obtained, which are presented in the sequence of images. These images offer a detailed perspective on how this complex and dynamic reaction unfolds.

vol. 30, issue 1 / 2024
pp. 58-67

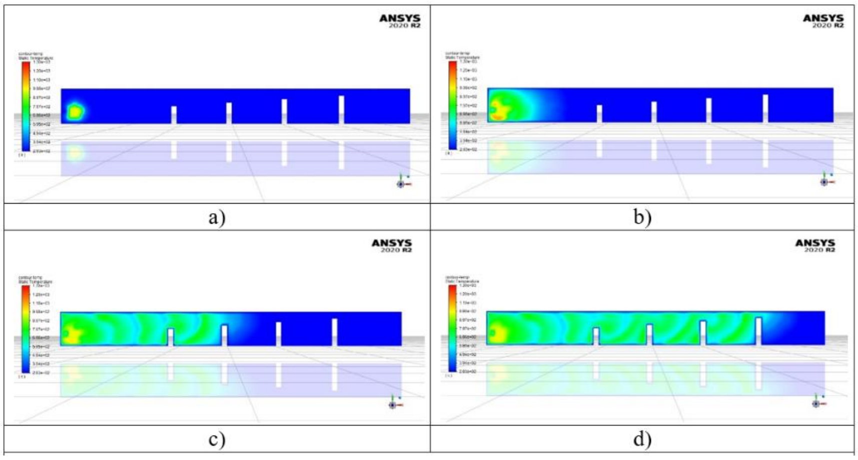


Fig. 4. Colour contours of temperatures

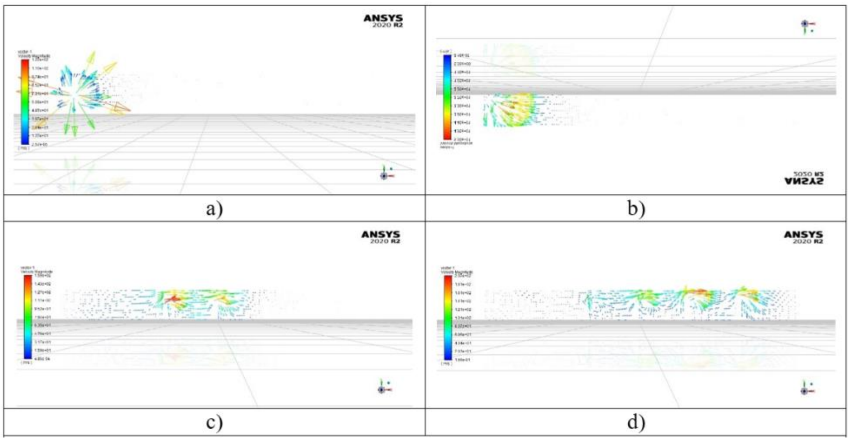


Fig. 5. Velocity vectors

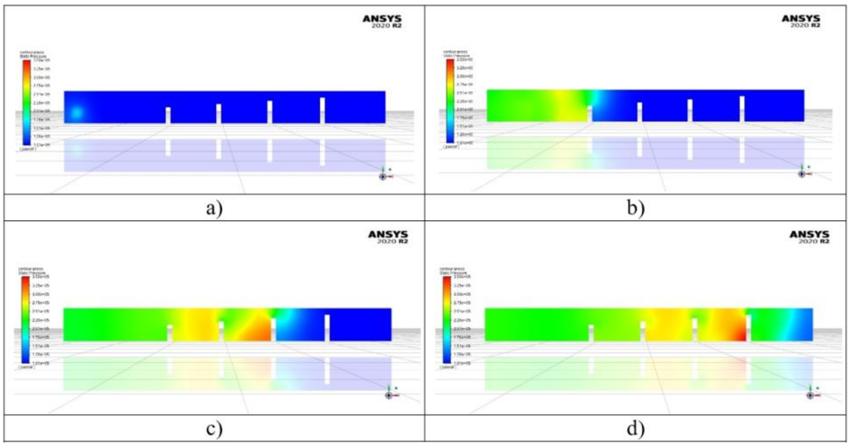


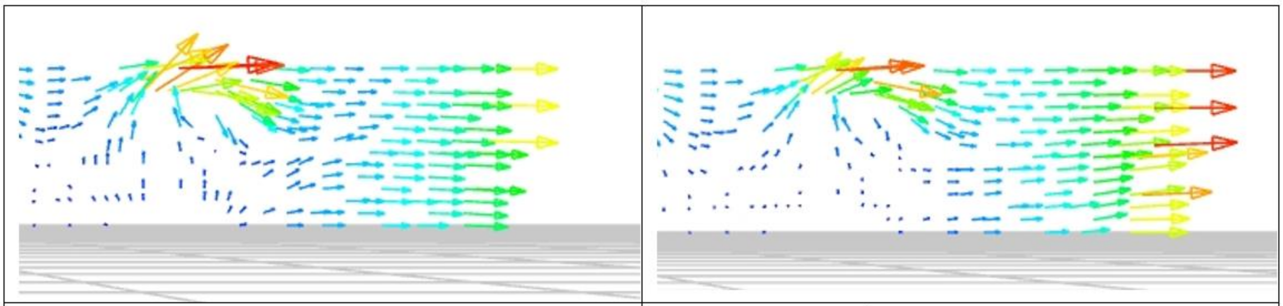
Fig. 6. Colour contours of the pressures

4. Results

In Figure 7, images obtained at two distinct moments are presented: t = 0.0014 and t = 0.0015 s. These moments coincide with the surpassing of the pressure threshold set by the User Defined Function (UDF). Furthermore, in Figure 7b), it can be observed that the velocity vectors are higher than those in Figure 7a), indicating a change in the system dynamics. This change suggests the opening of the tube end, thereby transforming that surface from a wall into a pressure outlet. This facilitates the release of explosion pressures.

The confirmation of this hypothesis is also observed in the behaviour of the pressure across the entire volume of the rectangular tube. Starting from the aforementioned moment, the pressures begin to decrease, and the curves show a tendency towards the atmospheric pressure value. This trend indicates that the explosion pressures are efficiently released from the system, and the tube returns to an equilibrium state under atmospheric pressure.

vol. 30, issue 1 / 2024
pp. 58-67



a) t = 0.0014 s	b) t = 0,0015 s

Fig. 7. Releasing explosion overpressures after exceeding the set threshold

Following the virtual simulation of the explosive mixture of air and methane, the results regarding the recorded pressures are detailed in the following table, covering the surfaces analysed in this study. These data provide a comprehensive perspective on the pressure distribution in various areas of the studied surfaces, offering essential information for evaluating and understanding the behaviour of the explosion in the enclosed space with obstacles.

Table 1. Pressures recorded in the computational simulation

Pressure volume [Pa]	Pressure Obstacle 1 [Pa]	Pressure Obstacle 2 [Pa]	Pressure Obstacle 3 [Pa]	Pressure Obstacle 4 [Pa]	Pressure end tube [Pa]	Time [s]
101325	101325	101325	101325	101325	101325	0
101327.4	101325.6	101325.6	101325.6	101325.6	101325.6	0.0001
101327.8	101326.1	101326	101326	101326	101326	0.0002
164918.4	101317.9	101314.6	101322.7	101325	101326	0.0003
173766.9	101444.5	101291.3	101340.3	101338.9	101332.1	0.0004
248451.7	104844.6	101225.1	101366.3	101380.8	101348.8	0.0005
285013.6	136571	101414.1	101394.5	101433.4	101381.9	0.0006
276967.5	267157.5	105874.5	101386.2	101469.3	101421.9	0.0007
325218.6	325218.6	152315.3	101802.8	101465.9	101463.6	0.0008
295130.3	268304.3	293728.6	108740.4	101463	101516	0.0009
345791.1	248614.4	345791.1	174074.9	102058.2	101525.9	0.001
317721.1	246412.3	277372	317721.2	110620.4	101522.2	0.0011
342291.9	246757.9	262316.3	342291.9	179913.8	101720.5	0.0012
319448	242679.5	258378.6	281426.3	319436.1	105027.7	0.0013
349716.8	236987	260713.3	271585.4	349716.8	138124.3	0.0014
297224	232262.2	259460.2	271492.5	283911.7	117319.1	0.0015
293259.3	229883.1	253792.3	273719.2	276447.1	110271.3	0.0016
286593.8	229837	247385.9	274135	276159.1	105384.4	0.0017
278250.4	230969.3	242371.8	270587.6	278249.6	101888.9	0.0018
275006.8	232672.5	239286.3	263842.1	275006.8	101325	0.0019
266410.6	234379.6	237613.8	256572.3	266410.6	101325	0.002
255137.6	235773.1	236879.3	249864.4	255137.5	101325	0.0021
245071.2	236810.9	237350.1	243728.7	243239.5	101325	0.0022
241069.6	237632.7	238283.6	238179.3	231861.3	101325	0.0023
240312.7	238358.1	238728.8	233903.2	221461.3	101325	0.0024
240681.5	239032.8	238552.1	229650.5	212099	101325	0.0025
240593.3	239618.9	237747.9	225380.5	203741.2	101325	0.0026
241115.4	240017.7	236343.1	221153.2	196425.4	101325	0.0027
242154.1	240126.1	234374.8	217084.1	190222.7	103689.3	0.0028
242756.7	239907.7	231963.7	213300.8	185262.8	103889.6	0.0029
243311.5	239291.8	229206.8	209846.8	181612.7	108328.6	0.003
243491.2	238285.5	226275.1	206776.7	179236.3	103973.8	0.0031
283868.7	276752.3	282895	281610.4	263587.2	104260.7	0.0032
285692.5	280560.9	287291.4	286352.6	268137.8	109449.3	0.0033
287516.2	284369.5	291687.8	291094.8	272688.3	106965.9	0.0034
289340	288178.1	296084.3	295837	277238.9	105868.2	0.0035

Pressure volume [Pa]	Pressure Obstacle 1 [Pa]	Pressure Obstacle 2 [Pa]	Pressure Obstacle 3 [Pa]	Pressure Obstacle 4 [Pa]	Pressure end tube [Pa]	Time [s]
291163.7	291986.6	300480.7	300579.2	281789.5	104559.2	0.0036
292987.5	295795.2	304877.1	305321.4	286340.1	104827.4	0.0037
294811.2	299603.8	309273.5	310063.6	290890.7	103445	0.0038
296635	303412.4	313670	314805.9	295441.2	102252	0.0039
298458.8	307221	318066.4	319548.1	299991.8	102055.5	0.004
300282.5	311029.5	322462.8	324290.3	304542.4	101941.9	0.0041
302106.3	314838.1	326859.3	329032.5	309093	101325	0.0042
303930	318646.7	331255.7	333774.7	313643.6	101325	0.0043
305753.8	322455.3	335652.1	338516.9	318194.2	102273.2	0.0044
307577.5	326263.8	340048.5	343259.1	322744.7	102780.3	0.0045
309401.3	330072.4	344445	348001.3	327295.3	104001.3	0.0046
311225	333881	348841.4	352743.5	331845.9	105233.6	0.0047
313048.8	337689.6	353237.8	357485.7	336396.5	103204.2	0.0048
314872.6	341498.2	357634.2	362227.9	340947.1	103435.7	0.0049
316696.3	345306.7	362030.7	366970.2	345497.6	104071.2	0.005
318520.1	349115.3	366427.1	371712.4	350048.2	104228.4	0.0051
320343.8	352923.9	370823.5	376454.6	354598.8	104348.1	0.0052
322167.6	356732.5	375219.9	381196.8	359149.4	103688.9	0.0053
323991.3	360541	379616.4	385939	363700	102512.1	0.0054
325815.1	364349.6	384012.8	390681.2	368250.5	101669.5	0.0055
327638.8	368158.2	388409.2	395423.4	372801.1	102508.1	0.0056
329462.6	371966.8	392805.6	400165.6	377351.7	101325	0.0057
331286.4	375775.4	397202.1	404907.8	381902.3	104232.8	0.0058
333110.1	379583.9	401598.5	409650	386452.9	104398	0.0059
334933.9	383392.5	405994.9	414392.2	391003.5	103575.5	0.006
336757.6	387201.1	410391.3	419134.5	395554	104202	0.0061
338581.4	391009.7	414787.8	423876.7	400104.6	105518.8	0.0062
340405.1	394818.3	419184.2	428618.9	404655.2	104097.9	0.0063
101325	398626.8	423580.6	433361.1	409205.8	105191	0.0064

5. Conclusions

In this paper emphasizes the importance of a mechanical spark with movement as an efficient source of ignition for the explosive atmosphere. This finding can contribute to enhancing safety measures by recognizing and mitigating potential ignition sources in real-world scenarios involving air-methane gas mixtures.

During the virtual simulation, the explosion of the air and methane mixture was represented within a tube containing obstacles of varying sizes, characterized by low resistance that yielded at a certain predefined pressure threshold, triggering explosion overpressures. The implementation of this simulation involved integrating files written in the programming languages C and SCHEME, enabling a detailed and precise analysis of the results.

By conducting simulations on real-scale virtual models within the context of potential gas explosion scenarios, a greater clarity regarding the underlying mechanisms of these events can be anticipated. These simulations provide an opportunity to investigate in detail how gases spread within a room, how they interact with glazed surfaces, and how the explosion evolves in an enclosed environment. The results of these simulations can bring a deeper understanding of the physical phenomena involved in such events and can serve as a basis for improving preventive measures and interventions in case of gas explosions in buildings and other enclosed spaces. Therefore, the use of real-scale virtual models represents a valuable tool for researching and managing the risks associated with these scenarios.

The results obtained through computerized simulation of virtual scale models can be extrapolated to real-world situations involving glazed surfaces, providing information about the potential impact and consequences of gas explosions in enclosed spaces.

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