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Numerical simulation of an accidental release of hydrogen in a filling station for hydrogen powered vehicles

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Abstract. In the current political-economic-social climate in which the governments of the countries of the world promote clean energy sources, hydrogen is one of the alternatives proposed to replace fossil fuels. That is why it is necessary to carry out the necessary research to establish the safety characteristics of hydrogen, using available computer modeling software. In this paper, the numerical simulation will be performed using the software package Fire Dynamics Simulator version 6.7.1. Taking into account technological development in the field of computing equipment, numerical simulations can be performed very well, and the results are very close to reality.

1 Introduction

Since the arrival of the age of steam engines in the mid-18th century, by James Watt, thus starting the first industrial revolution, necessitated the rapid extraction and burning of fossil fuels, which lead to the release of greenhouse gases into the atmosphere in quantities never seen before. In the chart below is the observed levels in total greenhouse gas concentration levels between 1900 and 2020 [1]

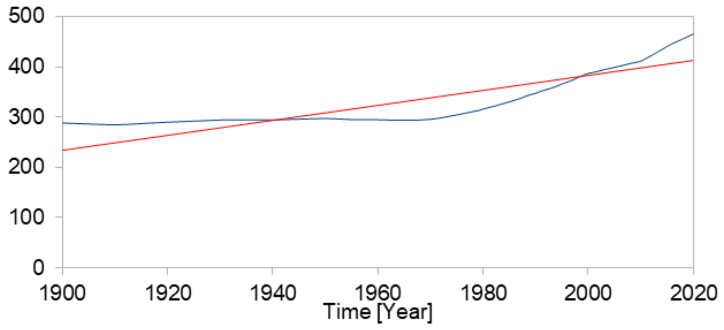

Fig. 1. Yearly greenhouse concentrations

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Due to the increase of the concentration of greenhouse gases in the atmosphere, the global temperatures continue to rise, leading to increase in a number of negative effects, such as drought, high intensity storms, rise of the sea level, melting of glaciers. This rise in global temperatures, is corroborated by a number of data collected at a global level. [2] In order to mitigate these negative effects of global warming it is necessary to transition the economy from the consumption of fossil fuels to other, more cleaner forms of energy.

In the current political, social and political climate, where the governments of the countries of the world promote clean energy sources, hydrogen is one of the alternatives proposed to replace fossil fuels. Due to the different thermal, chemical properties of hydrogen, compared to fossil fuels, it is necessary to conduct research to determine the behavior and potential risks the use of hydrogen presents in the ordinary activities.

In this paper we present a computer simulation of an accidental release of hydrogen at a filling station for hydrogen powered vehicles.

2 Computational tools used for the simulation

There are a number of computational software tools available, that we can use to perform a computational modeling of an accidental release of hydrogen.

One of these tools is the Fire Dynamics Simulator (FDS), which can be used to simulate both fires and atmospheric phenomena.

This program was developed through collaboration between the National Institute of Standards and Technology (NIST) in the United States of America and the VTT Technical Research Center in Finland.

This software tool is a CFD type application, which is optimized for the numerical modeling of low-velocity thermal fluids by solving Navier - Stokes equations, characterized by a Mach number lower than 0.3.

Viewing the modeling results through the FDS application is done through the SMOKEVIEW utility included in the same software application package [3].

The Navier–Stokes equation which is used by the Fire Dynamics Simulator, are useful because they describe the physics of many phenomena of scientific and engineering interest. They may be used to model many other naturally occurring physical phenomena, such as the weather, ocean currents, water flow in a pipe and air flow around a wing.

The Navier–Stokes equations, in their full and simplified forms, help with the design of aircraft and cars, the study of blood flow, the design of power stations, the analysis of pollution, and many other things. Coupled with Maxwell's equations, they can be used to model and study magneto-hydrodynamics. [4]

One of the major advantages of the application is the support for parallel processing on multiple computing stations by defining multiple computational domains.

3 Description of the simulation

The computer simulation consists of defining of the computational domain, by establishing of the dimensions and resolution of the simulation, generating obstacles, defining the initial conditions on the simulation.

The dimensions of the computational domain are 16 meters on the OX direction, 8 meters on the OY direction and 4 meters on the OZ direction.

The geometry of consists of a number of 35 OBST type items which is part of the solid structure of the filling station and the vehicle.

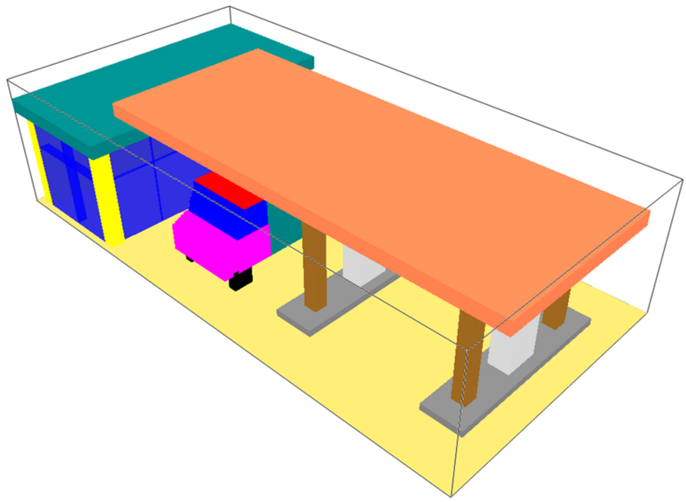

Fig. 2. Geometry of the computer simulation

The computational domain is connected to the exterior via 6 boundary items. One of the boundary items located at position Z = 0.0 meters, is set to be a closed type boundary item, representing the ground in which all the solid items within the computational domain rests. The rest of the boundary items are set to be open type boundary items, thus facilitating a better approximation of a real-world scenario.

The domain is split into a number of sub-domains, in order to facilitate running of the simulation in parallel on multiple computing processing cores. As such the domain was split into 64 sub-domains, each sub-domain with dimensions of 2,0 x 2.0 x 2.0 meters.

The resolution of the simulation, meaning the size of the cell, is set to 0,05 meters, thus each of these sub-domains containing a number of 64 000 cells, representing a total of 4 096 000 cells.

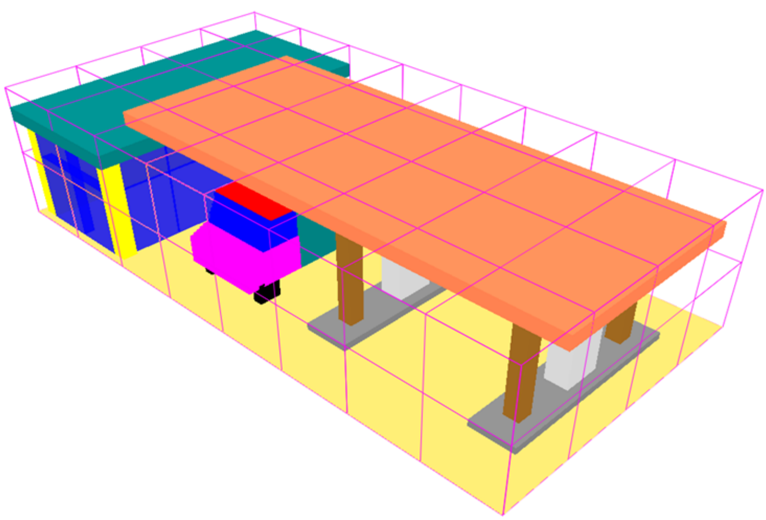

Fig. 3. Partitioning of the computational domain into multiple subdomains

To perform the computer simulation, some initial conditions are necessary to be defined, such as, the surrounding atmospheric temperature, atmospheric pressure, concentration of hydrogen gas, the size of the vent, the velocity of the escaping hydrogen gas, the duration of the simulation.

The values of these parameters are presented in the table below:

Table 1. Initial condition of the computer simulation

Parameter	Value	Unit
Ambient Temperature	20	C
Atmospheric Pressure	101 325	Pa
Vent Size	0.05 x 0.05	m
Gas Velocity	10	m/s
Gas Concentration	1	kg
Duration of Simulation	100	s

In order to record the results of the computer simulation, we have defined a number of data recording items such as SLICE items, which record data on a 2-dimensional plane, and a number of DEVC items which record the results at specific defined points inside of the computational domain.

Table 2. Position of the recording devices inside the computational domain

Sensor	Pos X [m]	Pos Y [m]	Pos Z [m]
1	08.50	04.00	00.50
2	08.50	04.00	03.00

Next, in the sequence of attached images, the evolution of the simulation is presented. In Figure 4 is presented the state of computer simulation inside of the computational domain at the beginning of the computer simulation. As it can be observed, the concentration of hydrogen gas is zero.

In Figure 5 is presented the distribution of the concentration of hydrogen gas. It can be observed that due to the specific properties of hydrogen, being lighter than air, raises upwards and potentially accumulates at the ceiling.

This tendency of hydrogen gas to accumulates at a higher elevation, is also presented by the data recorded by the sensors defined inside the computational domain.

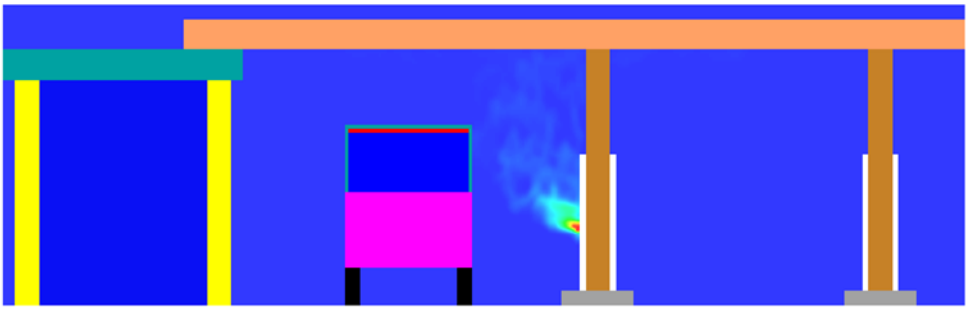

Fig. 4. State of the computer simulation at T = 100 sec.

In the next sequence of Figures, it is presented the evolution of the concentrations of hydrogen gas recorded by recording devices placed inside of the computational domain. The first sensor (Sensor 1) is placed at a height of 0.05 meters, and the data recorded by this sensor is presenter in Figure 5 below. Note that the red line in the chart below represents the mean value of the concentration of hydrogen gas recorded by Sensor 1.

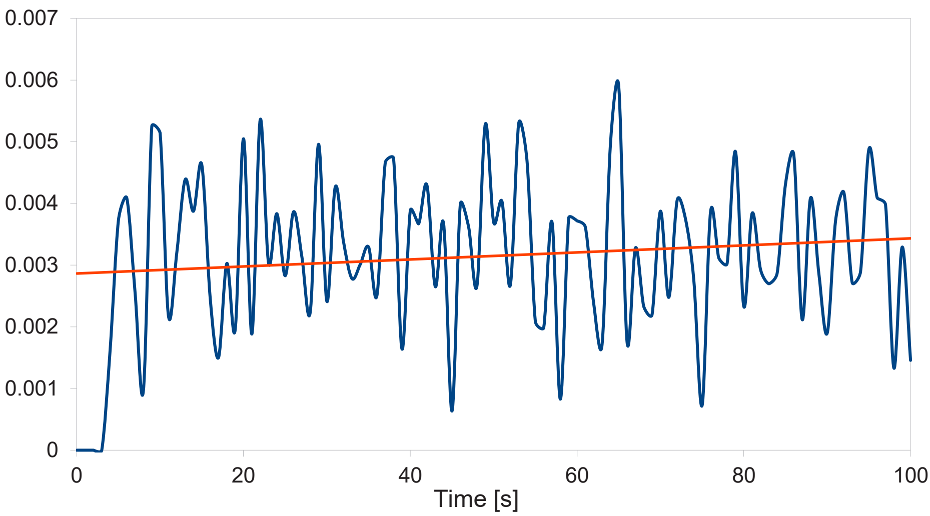

Fig. 5. Evolution of concentration of hydrogen gas recorded by Sensor 1

In Figure 6, below is presented the data recorded by the second sensor (Sensor 2), which is placed at a height of 3.00 meters. It can be observed that the value of the concentration of hydrogen gas fluctuates wildly, this can be explained by the interaction of hydrogen gas with the surrounding atmosphere, and with the solid obstacles present in the vicinity.
The red line in the chart below represents the mean value of the concentration of hydrogen gas recorded by Sensor 2.

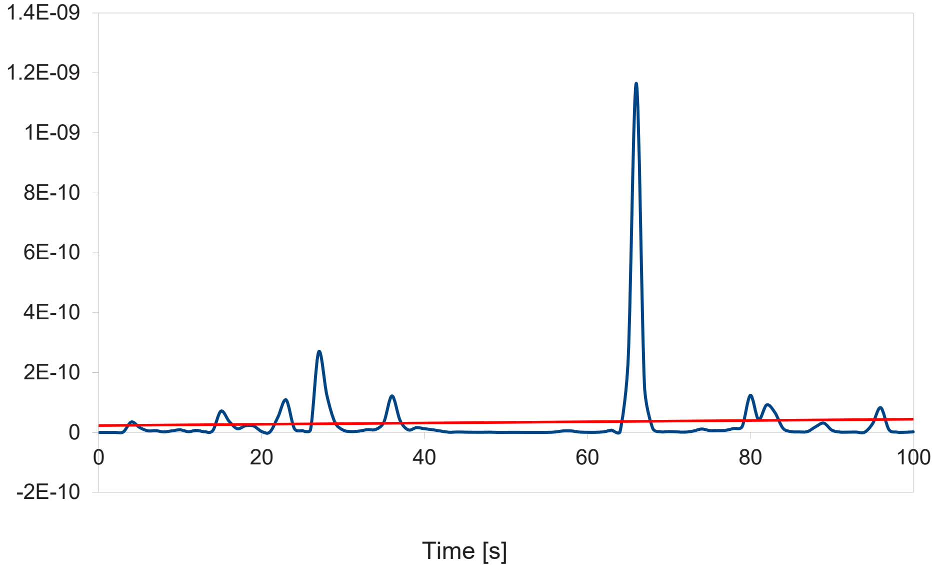

Fig. 6. Concentration of hydrogen gas recorded by Sensor 2

Comparing the values recorded by the two sensors, we can conclude that the concentration of hydrogen gas is higher at a higher elevation, due to the specific property of hydrogen of being a lighter than air gas. This property of hydrogen forces it to rise up, thus explaining the difference between the recorded values.
From the point of view of hydrogen being lighter than air, has similar behavior to other gases that are lighter than air such as methane.

3 Conclusion

By conducting this computer simulation of hydrogen escaping from a filling station, we can conclude that even with the benefit of the hydrogen as an 100 % clean fuel, the risks to safety remains high, thus taking appropriate measures to protect against explosions, is necessary.

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