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CFD modeling of subsonic and sonic methane gas release and dispersion

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ABSTRACT

In the event of a flammable liquid, gas, or vapor release the first step is to identify the type of outflow, which can fall into two categories sonic or subsonic. The two types of outflows carry different flow characteristics, which effect on the extent of the potentially explosive areas. In case of subsonic outflow, a short jet is formed without turbulent flow conditions at low velocity, which appears more concentrated around the source of release. With sonic outflow, a high velocity jet is formed with turbulent flow properties, which can extend further away from the source of release. The simulations examine the lower explosion limit of the flammable medium around the vessel where LEL20% or LEL40%. In addition, high temperature methane gas release was also presented.

KEYWORDS

computational fluid dynamics, explosive atmosphere, hazardous area classification, methane, lower explosive limit, expansion

1. INTRODUCTION

In industrial plants, where flammable materials are stored, produced, or processed, hazardous explosive atmospheres can occur, what could be one of most dangerous [1]. An analysis of chemical accidents between 1998 and 2015 showed that gas explosions are the most dangerous [2]. A gas explosion, which can be identified with the concept of explosion, Keller et al. [3] describes a process where a rapid rise in temperature and pressure occurs that causes an audible, spherically propagating pressure surge that results in oxidation or other exothermic reactions due to the explosion.

A distinction can be made between a continuous, voluminous gas cloud and an instantaneous accidental, volumetrically negligible release, where an explosion can only occur in the event of immediate ignition [4]. In these cases no gas explosion occurs, but rather only deflagration resulting in overpressurisation [5]. The severity of explosions depends on the position and strength of the ignition source, the volume and concentration of the gas or vapor cloud mixed with air [4]. In addition, the explosion is also influenced by the surrounding cascade and the combustion and explosive properties of the combustible material [6].

The possibilities of chemical plants accidents can be reduced by preliminary investigations HAZard and OPerability (HAZOP) [7], which include a detailed assessment of the potential consequences. Properly selected safety equipment and organizational measures also reduce the risk (explosion-proof equipment, fire and explosion protection regulations). Experimental assessments are instructive, however, such experimental predictive assessments are limited to small-scale accidents, as replicating large-scale explosions would be very costly, time-consuming and dangerous [8].

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Cost and safety optimization [9] in mind have led to the rapid development of more practical theoretical models. The Computational Fluid Dynamics (CFD) and others software may include the following:

- ANYSY (CFD simulation) [10–12];
- Arial LOcation Hazardous Atmosphere (ALOHA) [13];
- GEXCON FLame ACceleration Simulator (FLACS-CFD) [14, 15];
- DNV PHAST [16];
- TNO Effects [17].

The safe and effectively cheaply reproducible software environment provided by the simulations has great advantages, which is still extensively used nowadays for initial screening validation purposes [18]. Researchers typically validate their simulation results with investigations data or other experience [19–21]. Interesting and useful simulation studies were evaluated with the help of the CFD. Papanikolaou and Baraldi [20] study of high-pressure hydrogen gas propagation in an external environment. In a test space in an external environment, the different air flow speeds can also greatly influence the spread of explosive gases [21]. In the analyzes an important aspect is the relative density of the gas, based on which it can spread better upwards or downwards. This phenomenon can be investigated excellently with simulations [22]. Natural gas contains approximately 95% methane, one of the dangerous substances that can be present anywhere in everyday life. Its spread in the external environment in a large area Sebastian et al. was examined in his study [23].

2. THEORETICAL BACKGROUND

Literature and standards are available to identify these hazardous areas [24, 25]. The result of hazardous area classification reveals the type and extent of potentially explosive areas. In the event of a flammable liquid, gas or vapor release the first step is to identify the type of outflow, which can fall into two categories sonic or subsonic [26]. To determine the type of outflow the critical pressure of the medium must be calculated, however in case of unknown parameters 1.89 bar can be used as the average value of critical pressure. If the internal pressure is lower than the critical pressure it is classified as subsonic flow, otherwise it is sonic outflow.

The two types of outflows carry different flow characteristics, which affect the extent of the potentially explosive areas. In the case of subsonic outflow, a short jet is formed without turbulent flow conditions at low velocity, which appears more concentrated around the source of release.

With sonic outflow, a high velocity jet is formed with turbulent flow properties, which can extend further away from the source of release.

To decide the type of outflow, the critical pressure of the closed system must be determined. The expanding gas velocity is sonic (choked) if the internal pressure of the system is greater than the critical pressure, whereas it is subsonic (no choking) if the internal pressure of the system is less than the critical pressure. According to ILNAS-IEC 60079-10-1:2015 [25], the determination of the emission rate of gases or vapors is an important condition for proceeding with calculations, as different relationships have to be applied in the subsonic and sonic cases. The first step is to determine the adiabatic expansion polytrophic index of the gas or vapor according to Eq. (1):

$$\gamma = \frac{M \cdot C_p}{M \cdot C_p - R}, \tag{1}$$

where M is the molar mass [kg·kmol^{-1}]; C_p is the specific heat capacity [J·kg^{-1}·K^{-1}]; and R is the universal gas constant [J·kmol^{-1}·K^{-1}]. Eq. (1) gives $\gamma = 1.3$ for methane. The critical pressure value can be determined by Eq. (2):

$$p_c = p_a \cdot \left(\frac{\gamma + 1}{2} \right)^{\frac{\gamma}{\gamma - 1}}, \tag{2}$$

where p_a is the molar mass [Pa]; γ is the adiabatic expansion politropic index [-]. Eq. (2) gives $p_c = 185\ 904$ Pa for methane.

3. RESULTS AND DISCUSSION

The ANSYS CFD were simulated the propagation of the two types of emission through a source of release located on a methane tank. The results were presented the outflow and spreading of the slower and more concentrated subsonic outflow and the high velocity, but less concentrated sonic outflow. Both subsonic and sonic transient state simulations were performed using a large vortex model k–ω Shear Stress Transport (SST) with polyhedral mesh. Material properties were determined using the Peng-Robinson correlation. There is no airflow both simulations. The rate of emissions was also determined using a mathematical model.

3.1. Subsonic release

The mathematical relationship proposed by ILNAS-IEC 60079-10-1:2015 [25] for the quantification of subsonic emissions given by Eq. (3), which also applies the adiabatic expansion politropic index of Eq. (1):

$$W_g = C_d \cdot S \cdot p \cdot \sqrt{\frac{M}{z \cdot R \cdot T} \cdot \frac{2 \cdot \gamma}{\gamma - 1} \left[1 - \left(\frac{p_a}{p} \right)^{\frac{\gamma}{\gamma - 1}} \right]} \cdot \left(\frac{p_a}{p} \right)^{\frac{1}{\gamma}}, \tag{3}$$

where C_d is the discharge coefficient [-]; S is the hole cross section [m^2], which represents a hole with a diameter of 0.01 m as the source of release; p is the internal pressure of medium [Pa]; z is the compressibility factor [-]; T is the temperature of medium [K]. According to the boundary conditions of the variables $C_d = 1.0$, $S = 0.000078$ m^2, $p = 180{,}000$ Pa, $z = 1.0$, $T = 298.15$ K, the mass release rate of methane: $W_g = 0.024$ kg s^{-1}.

The simulation duration examined was 4 s, which required 7.5 days of run time. Between the start and end points of the period under study, the level of gas emissions was monitored. As it is shown in Fig. 1 the gas emission rate decreases with time, as the pressure inside the tank decreases accordingly. Fig. 1 shows that the simulation proves a lower value.

During the simulation, the methane gas propagation states are shown before the methane tank and between the operating building and other tank in Figs 2–4 at time instants of 0.5 and 4.0 s. The tested concentrations of the Lower Explosion Limit (LEL) are 20 and 40%.

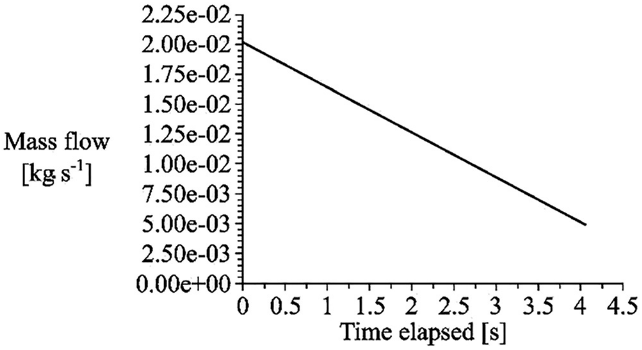


Fig. 1. Time series function of the subsonic emission

The LEL 20% value for methane is 0.88 volume percent (vol%). Initially a longer jet is visible, then after deceleration the gas volume spreads out and can penetrate into an area below ground level due to the effects of expansion. At LEL 40%–1.76 vol% a little thinner both cases. The length and extent of the LEL-4.4 vol% increases over time.

3.2. Sonic release

The mathematical relationship proposed by ILNAS-IEC 60079-10-1:2015 [25] for the quantification of sonic emissions is given by Eq. (4), which is almost identical to Eq. (3),

$$W_g = C_d \cdot S \cdot p \cdot \sqrt{\frac{M}{z \cdot R \cdot T} \cdot \left(\frac{2 \cdot \gamma}{\gamma + 1}\right)^{\left(\frac{\gamma+1}{\gamma-1}\right)}}. \qquad (4)$$

According to the boundary conditions of the variables almost same than subsonic, the internal pressure of the medium is higher, exactly $p = 600{,}000$ Pa. The mass release rate of methane: $W_g = 0.08\ \mathrm{kg{\cdot}s^{-1}}$.

The simulation duration examined was 10.5 s, which required 18 days of run time. Based on preliminary calculations, it takes approximately this time and a little more to empty the tank. Between the start and end points of the

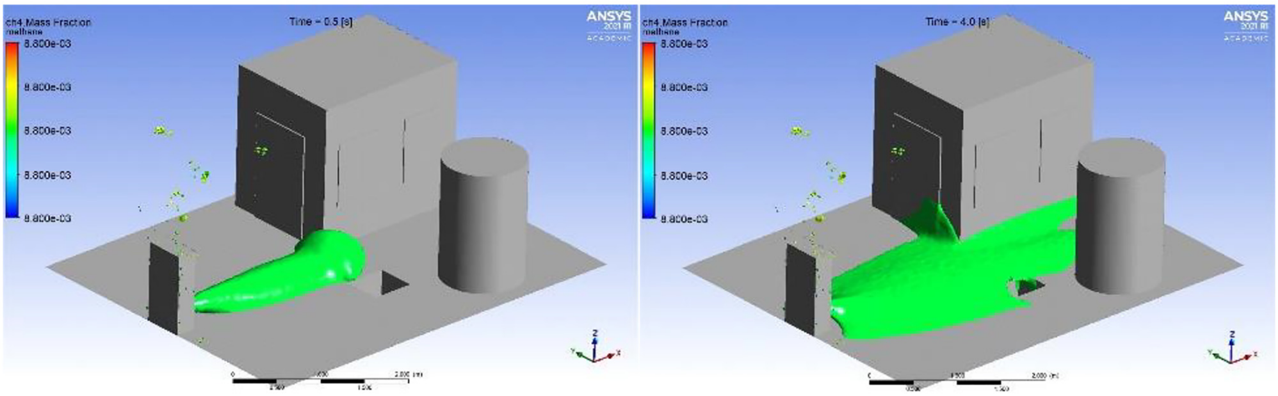


Fig. 2. Surfaces reaching LEL 20% in 0.5 s (left), 4.0 s (right)

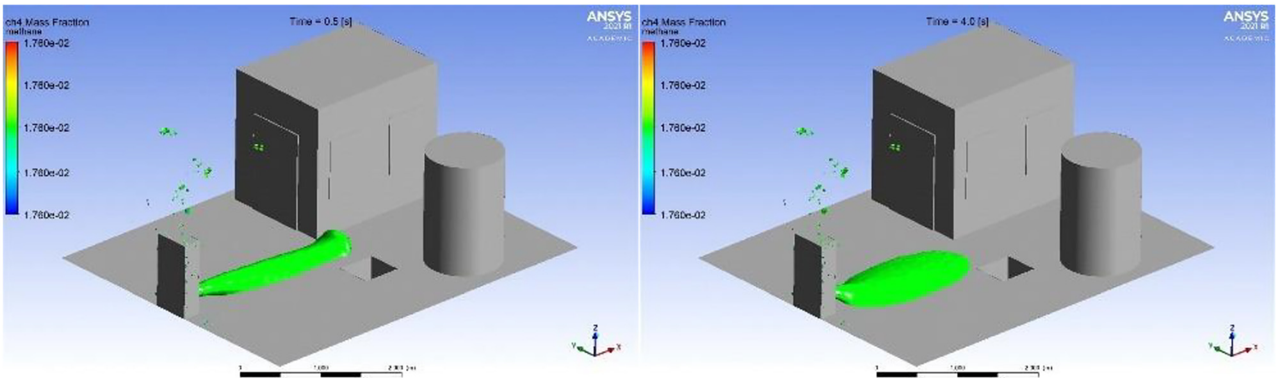


Fig. 3. Surfaces reaching LEL 40% in 0.5 s (left), 4.0 s (right)

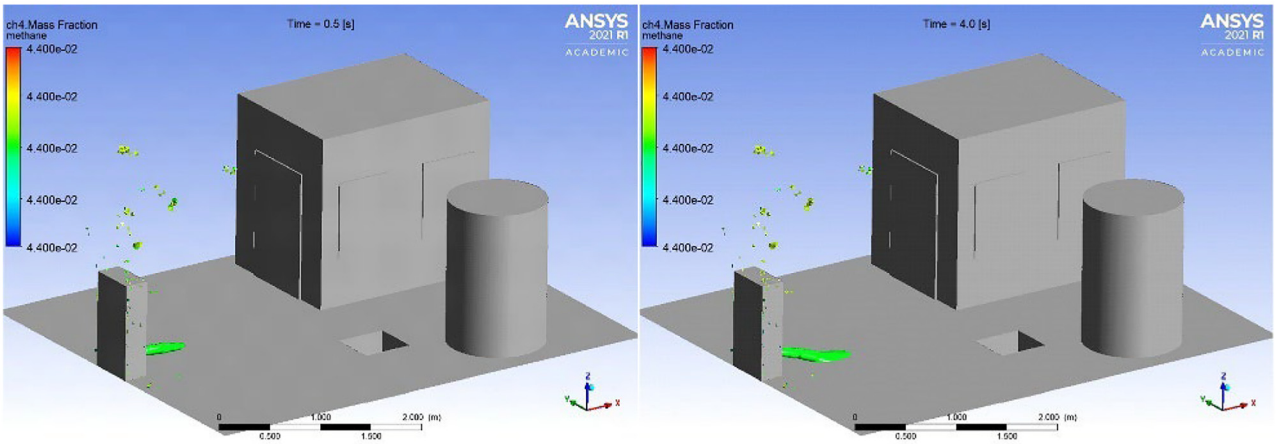


Fig. 4. Surfaces reaching LEL in 0.5 s (left), 4.0 s (right)

period under study, the level of gas emissions was monitored. As it is shown in Fig. 5 the gas emission rate decreases with time, as the pressure inside the tank decreases accordingly. The figure shows that the simulation shows a lower value.

During the simulation, the methane gas propagation states are shown before the methane tank and between the operating building and other tank in Figs 6–8 at time instants of 0.5 and 8.0 s at the same concentrations as subsonic. At 8.0 s the gas emission is close to a steady state, it is not necessary to look at the last simulated moment.

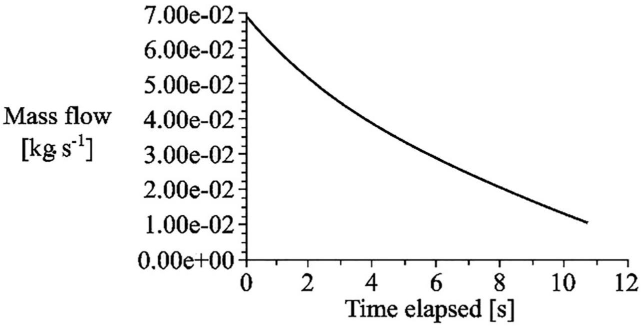


Fig. 5. Time series function of the sonic emission

At LEL 20% - 0.88 vol% are the same effects when the methane can penetrate into an area below ground level due to the effects of expansion. At the LEL - 4.4 vol% in the sonic case the LEL volume decreases. The high velocity causes fresh air to flow in a vortex over the surface of the volumes, diluting the concentration of the medium. It is the eddy diffusion [27] (see Fig. 9). In both outflows, the distance and location of the objects affected the direction of propagation as obstacles. Different distances and positions would result in different propagation forms.

3.3. High temperature medium release

In addition to investigating the propagation, the temperature variation of the outflow medium is simulated because of the lower explosion limit depends on the temperature of the medium [28] (the higher the lower). The results of the simulations shown in Fig. 10 indicate that a methane medium at 80 °C cools down very quickly in 1 s, both in subsonic and sonic outflow.

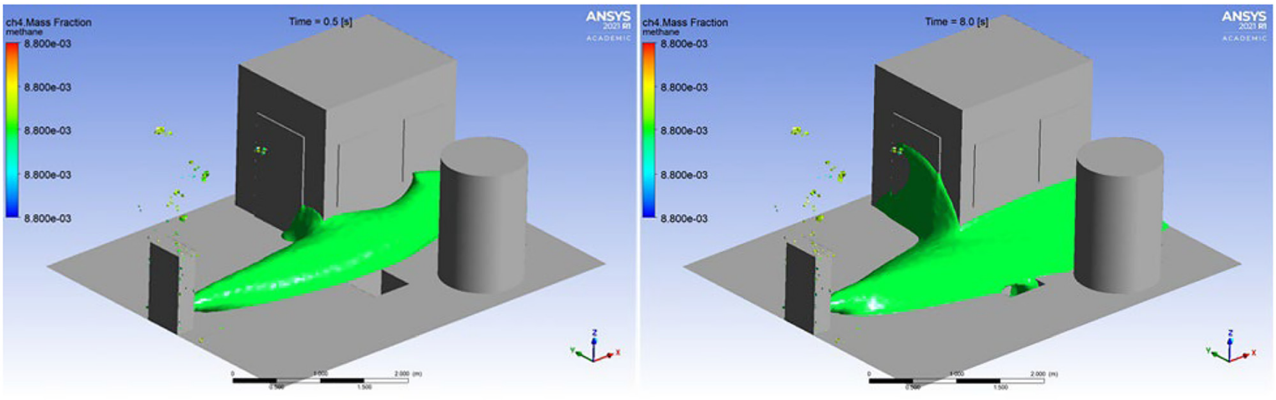


Fig. 6. Surfaces reaching LEL 20% in 0.5 s (left), 8.0 s (right)

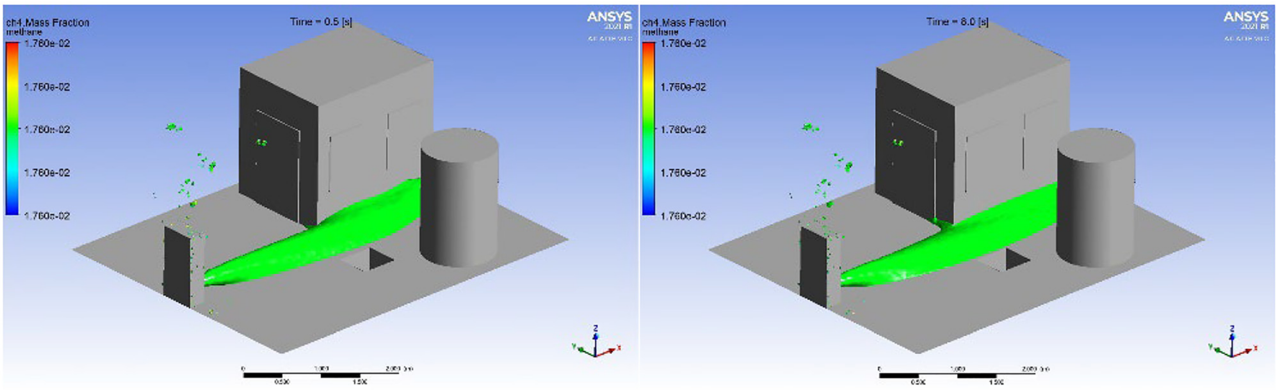


Fig. 7. Surfaces reaching LEL 40% in 0.5 s (left), 8.0 s (right)

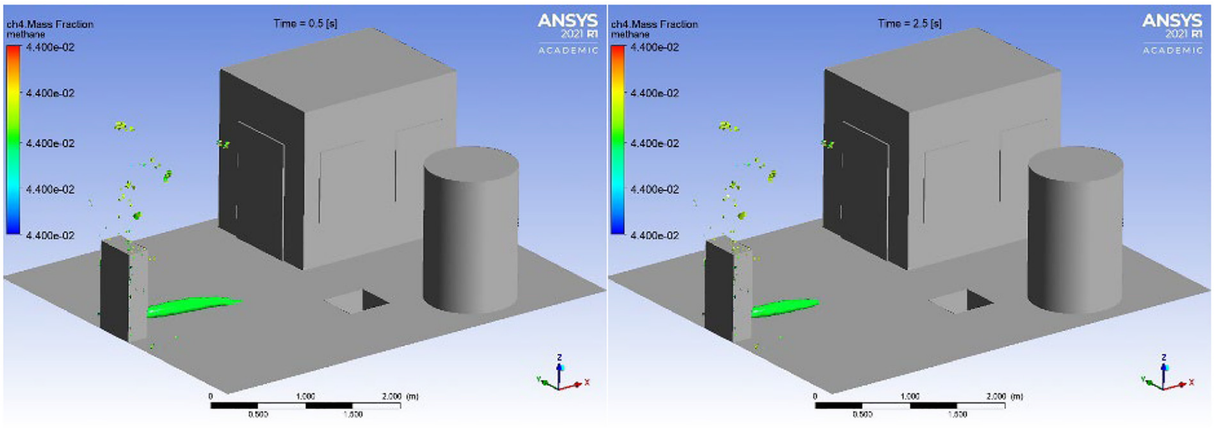


Fig. 8. Surfaces reaching LEL in 0.5 s (left), 8.0 s (right)

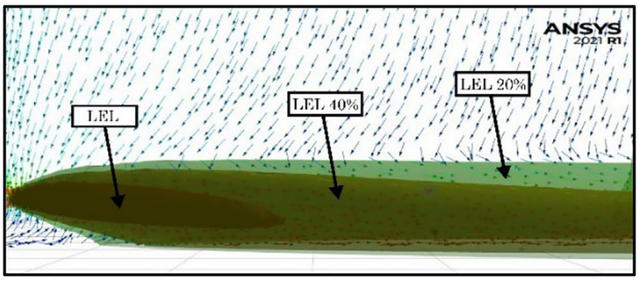
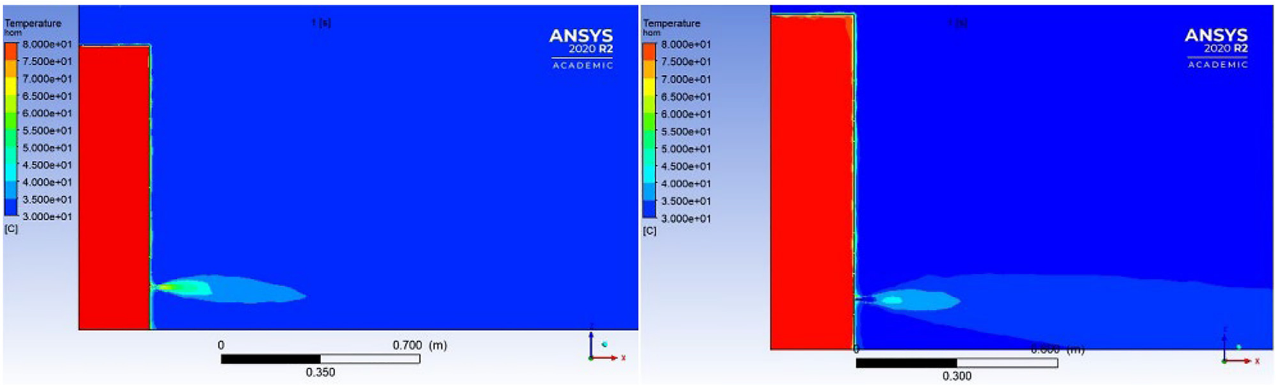


Fig. 9. Eddy diffusion

4. CONCLUSION

The use of simulation is a more accurate approach but requires more time. Mathematical relationships make higher emission values and larger zone but it means deviate conservatively, towards safety. At 20% of the lower explosive limit for both releases, lighter-than-air gas can penetrate to lower ground levels. Long or flattened beams are observed at 40% of the lower explosion limit. In the case of the lower



a) b)

Fig. 10. a) Subsonic, b) sonic outflow of 80 °C methane

explosion limit, an interesting phenomenon is observed, at subsonic the volume increases with time, in the sonic case it decreases. The temperature of the medium in the external space drops to low temperatures very quickly, the danger of correlating the explosion temperature with the temperature is not really there, although it may be significant at very high temperatures. In the future the simulations with measurements is planed to validate.

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