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FORMATION OF CRITICAL CONCENTRATIONS OF NATURAL GAS AT ITS LEAKAGE

Spreading of natural gas during its leak from a domestic low pressure pipeline in a confined space is a complicated issue depending on many factors. In relation to possible explosion, created dangerous concentrations could be identified effectively by numerical simulations using mathematical CFD models. It is suitable to verify the results of numerical simulations by real experiment, even if it is a simplified one. Verified mathematical model could then offer detail picture of spreading of gas in a whole focused space. In executed numerical analysis, several mathematical models of gas flow were applied and they were compared to the results of experimental measurements. This paper deals also with formation and propagation of critical concentrations of natural gas in the whole observed space in the cubical experimental chamber. All above-mentioned matters could be applied in the fields dealing with safety of persons, technologies and objects, and it could be also used for explanation of accidents related to leakage and explosion of gas.

Keywords: *CFD models, leakage of gas, propagation of gas, natural gas, dangerous concentration, explosive concentration.*

1. Introduction

At present number of incidents, in which gas exploded in residential homes, increases. From the viewpoint of safety it is important to identify places where dangerous and explosive concentrations can be created. Determination of the amount of combustible gas leaked from a broken installation gas pipework is most often performed using simplified calculations [1]. The time required for creation of an explosive concentration is also determined in a similar manner.

CFD numerical simulations [2] are an appropriate means for more detailed determination of propagation parameters of dangerous gas. This paper is devoted to the mathematical modelling of leakage and diffusion of natural gas using the software ANSYS Fluent [3 and 4]. Emphasis is also placed on verification of the accuracy of calculation, which is ensured by comparison of the data obtained from numerical simulations with experimental measurements.

2. Description of measuring system and of calculation

For simulation of leakage and diffusion of gas throughout the enclosed space we created a measuring system consisting of a gas pipeline damaged in a defined manner, of partly closed container and of detectors. Leakage of gas occurred from the samples with leaks prepared in advance (circular and elongated hole, cut on the hose, etc.).

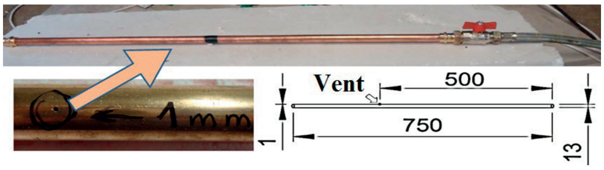

Fig. 1 Sample with a hole (mm)

Mathematical modelling considered a hole with diameter of 1 mm (Fig. 1) which was drilled into the copper gas pipe (sample). Area of the hole was 0.785 mm^2 and the pipe wall thickness was 1 mm. The sample (Fig. 1) with a hole was on one side blinded and from the other side it was connected to the installation low-pressure gas pipework.

The sample geometry (Fig. 2), designed with use of the software DesignModeler, consists only of inner volumes. The hole in gas pipeline was simulated by creation of a cylinder with the height and diameter of 1 mm on the inner volume of the sample.

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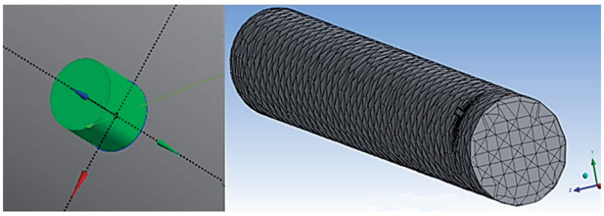

Fig. 2 Inner volume of the hole and calculation mesh of the sample

Mesh of the sample (Fig. 2), created in the software ANSYS Meshing, consists of 40 807 elements.

The gas leaked into an enclosed space (cubic vessel) with volume of approx. 1 m^3 [5]. A hole was cut into the vessel bottom in order to achieve during measurement a constant pressure in the vessel which would be identical to the pressure outside the vessel. Hardened polystyrene was used as construction material. Cubic vessel and location of the sample is shown in (Fig. 3).

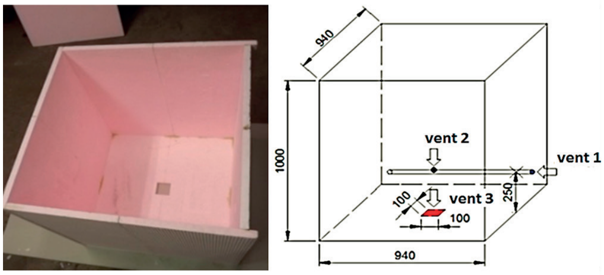

Fig. 3 Inner volume of the vessel and location of the sample (mm)

For easier creation of the calculation mesh the vessel geometry was formed from five connected volumes (Fig. 4).

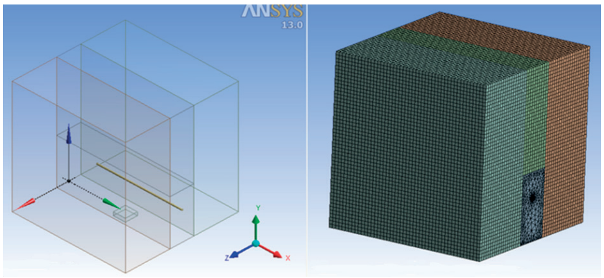

Fig. 4 Geometry of the whole system (on the left) and calculation mesh of the whole measuring system (on the right)

The whole computational mesh consists of 274 426 elements. The parameter for **determination of quality of a 3D cell** (degree of its deformation) is **0.748**. Limit value of the parameter is **0.9**. Quality of this computational mesh is therefore **satisfactory**.

Two stage detectors of inflammable gases CH4-GC20N, which were in-built into the walls of the created vessel, were used for detection of the flowing natural gas. Figure 5 illustrates position of detectors and tracepoints (dimensions are in millimetres).

During measurement we monitored times when 0.5% a 1% voluminal concentrations of methane were reached at the detectors' sensors. The measurement was finished after detection of 1% concentration by the last sensor. Each measurement was repeated three times. In the case of great difference of results the number of repeated measurements was increased as needed.

The function of six sensors used for experiment was ensured by six tracepoints created in the geometry of mathematical simulation. Position of points (black crosses) is the same as position of methane detectors in-built into the walls of the measuring system, which delimitates the space of gas leakage (Fig. 5). The program Fluent then evaluated on the basis of these points the dependence between the time of leakage and methane concentration in the mixture with air in voluminal percentages.

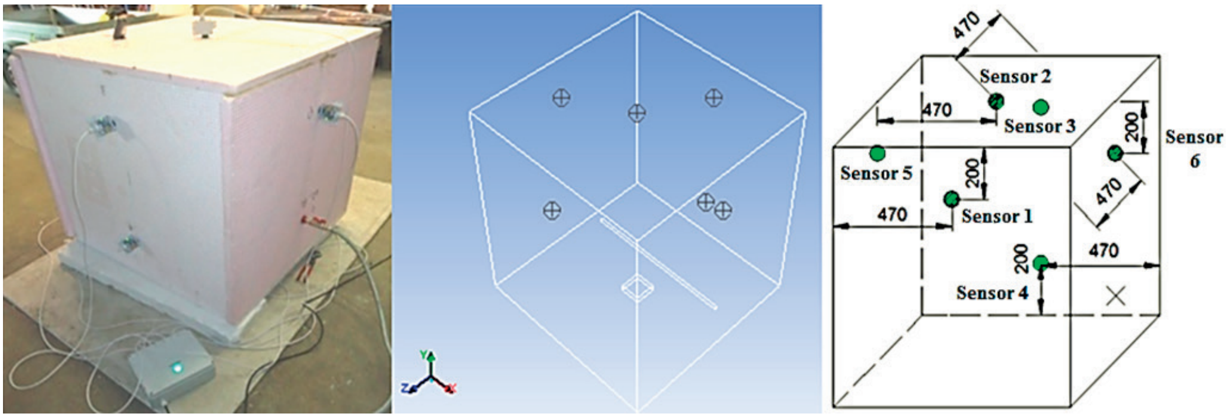

Fig. 5 Position of detectors and of tracepoints (mm)

3. Mathematical model of flow

The program ANSYS Fluent [3] for mathematical modelling of physical measurement was used. The basic relation used by the program for calculations is the **continuity equation** [4].

$$\frac{\partial(\rho)}{\partial}+\frac{\partial(\rho u_x)}{\partial x}+\frac{\partial(\rho u_y)}{\partial y}+\frac{\partial(\rho u_z)}{\partial z}=S_z$$

Simulation of methane flow through the space uses the **Navier-Stokes' equations** [4],

$$\frac{\partial\rho u_x}{\partial t}+\frac{\partial\rho u_x u_x}{\partial x}+\frac{\partial\rho u_y u_z}{\partial y}+\frac{\partial p u_z u_z}{\partial z}=$$

$$\rho a_x-\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left(\mu\frac{\partial u_x}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial u_x}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial u_x}{\partial z}\right)+S_x$$

$$\frac{\partial\rho u_y}{\partial t}+\frac{\partial\rho u_x u_y}{\partial x}+\frac{\partial\rho u_y u_y}{\partial y}+\frac{\partial p u_z u_y}{\partial z}=$$

$$\rho a_y-\frac{\partial p}{\partial y}+\frac{\partial}{\partial x}\left(\mu\frac{\partial u_y}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial u_y}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial u_y}{\partial z}\right)+S_y$$

$$\frac{\partial\rho u_z}{\partial t}+\frac{\partial\rho u_x u_z}{\partial x}+\frac{\partial\rho u_y u_z}{\partial y}+\frac{\partial p u_z u_z}{\partial z}=$$

$$\rho a_z-\frac{\partial p}{\partial z}+\frac{\partial}{\partial x}\left(\mu\frac{\partial u_z}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial u_z}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial u_z}{\partial z}\right)+S_z$$

By combining the above mentioned relations it is possible to determine pressures and velocities depending on all three coordinates (x, y, z) in the whole calculation mesh for each time step.

At solution of propagation of admixtures it is necessary to resolve local mass fractions of admixtures ”$Y_{i'}$“ [-] in the mixture,

$$Y_{i'}=\frac{m_{i'}}{m}=\frac{\rho_{i'}V_{i'}}{\rho V}=\frac{\rho_{i'}}{\rho}\alpha_{i'},$$

where $m_{i'}$ [kg] is mass of the admixture *i´*; *m* [kg] is total mass of the mixture; $\alpha_{i'}$ [-] is voluminal fraction of the admixture *i´* in the mixture.

Transfer of admixtures (of mass fraction) is resolved by the **balance equation** [4] which in the changing time calculates with the values of mass fractions of the admixture ”$Y_{i'}$“ and with components of velocity of flow of present gases ”u_i“.

$$\frac{\partial}{\partial t}(\rho Y_{i'})+\frac{\partial}{\partial x_j}\cdot(\rho u_j Y_{i'})=-\frac{\partial}{\partial x_j}J_{i',j}+R_{i'}+S_{i'}$$

”$J_{i',i}$“ is diffusion flow of the i^{th} component of the mixture, ”R_i“ is the net rate of production of species *i* by chemical reaction and ”S_i“ is the rate of creation by addition from the dispersed phase plus any user-defined sources.

In the solved task a transition occurs between laminar and turbulent flow. It is a transition region where flow in the pipeline is laminar (Re = 359), while in the zone of leaks the flow is, on the contrary, turbulent as a result of big increase in speed (Re = 4 640).

In order to achieve the best possible agreement of numerical simulation with the experimental measurement we used six mathematical models of flowing (”**Laminar**“; **”k-ε“**; **”k-ω“**). In the model**”k-ε“** we tested the variants **k-ε Standard; k-ε RNG** and **kε** Real**izable**. In the model **”k-ω“** we tested the variants **k-ω Standard and k-ω SST** [4].

For solution of above equations method of control volume was used.

4. Agreement of numerical simulation with physical experiment

Experimental part deals with propagation of natural gas into free space. It is, therefore, necessary to define in simulation that this is a mixture of natural gas with air. Database of the program Fluent contains only the mixture of air and methane [3]. It is possible to add other components of natural gas. This step would probably slow down the calculation due to higher number of unknown quantities and thus of calculated equations.

The used Transit natural gas contains 98.39 % of methane [6]. By comparison of densities of methane from the program database ($\rho_{27°C}$ = 0.6679 [kg/m^3]) and of Transit natural gas from literature [6] ($\rho_{20°C}$ = 0.680; $\rho_{30°C}$ = 0.658 [kg/m^3]) we can see a very good agreement. Thanks to these facts it is possible to consider this simplification to be acceptable.

Before describing propagation of gas in an enclosed space it was necessary to verify correctness of numerical simulation. The diagrams below present the results of six mathematical models with modifications approaching best the real flowing, which were compared with measurements. Diagrams in figures show dependence of the change of concentration on response time in the detectors Nos. 2 and 4 (Fig. 6 and Fig. 7).

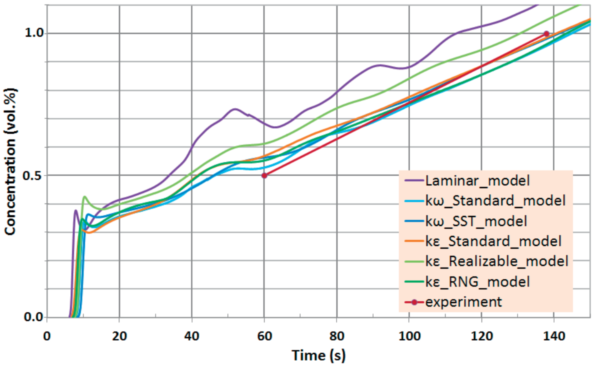

Fig. 6 Dependence of concentration change on response time of the sensor No. 2 [5]

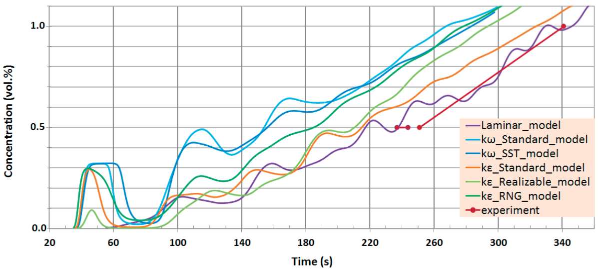

Fig. 7 Dependence of concentration change on response time of the sensor No. 4 [5]

It can be generally seen from the results that concentration first steeply increases and approximately at achievement of 0.3% to 0.5% of concentration the methane concentration further smoothly increases at tracepoints. Only at the fourth tracepoint the concentration steep increase again steeply decreased. After elapsing of several seconds it started again to increase smoothly. At the tracepoint No. 4 we can also observe a slight drop of concentration right before achievement of the 0.5% of concentration (model k-ε standard) and after it (laminar model). This phenomenon agrees with the measurement since at some measurements really only a glimmer took place and only after a while the diode signalling concentration of 0.5 % started to be lit permanently (Fig. 7).

5. Propagation of methane in an enclosed space

For the next evaluation of methane propagation through the space we took into account only the mathematical model „k-ε Standard“. This model was chosen due to its best agreement with the experiment.

Leakage of methane is visible on two created surface (sections through the whole calculation system). It is the surface on the axis ”z“ which passes through the centre of the pipeline, and surface on the axis ”x“ which intersects the centre of the hole from which methane leaks into the vessel. Range of the plotted contours, shown on created surfaces, is 0.5 to 1 vol. % concentration. The evaluation is, furthermore, completed with location of voluminal concentration 0.5% (blue) and 1% (red) in space.

Figure 8 shows direction of gas propagation during experiment. The hole was turned under the angle of 45°, that’s why methane propagated first to the detector No. 1 which signalled formation of 0.5% voluminal concentration. The gas then propagated along the wall to the top of the vessel. As soon as methane reached the top, it started to propagate to side walls, containing the detectors Nos. 5 and 6. Shortly after reaction of the first stage of the detector No. 2 (concentration of 0.5%), the velocity of gas propagation along the top of the vessel considerably dropped. On the rear wall (wall with detector No. 3) the flow of natural gas swirled. It is evident from the right bottom corner of the image (Fig. 9) that methane did not propagate along both side walls in a uniform manner. Methane flow, propagated along the right top part of the rear wall, reached the sensor No. 3 much more quickly than the gas flowing from the other side.

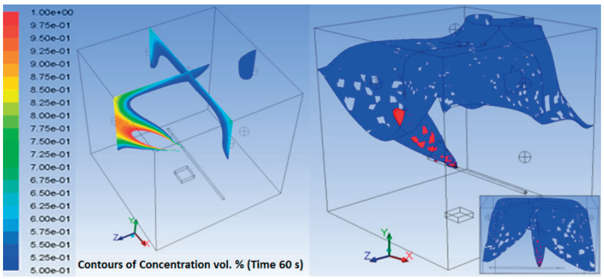

Fig. 9 Local concentrations during reaction of the sensor No. 3 (0.5 vol. %) [7]

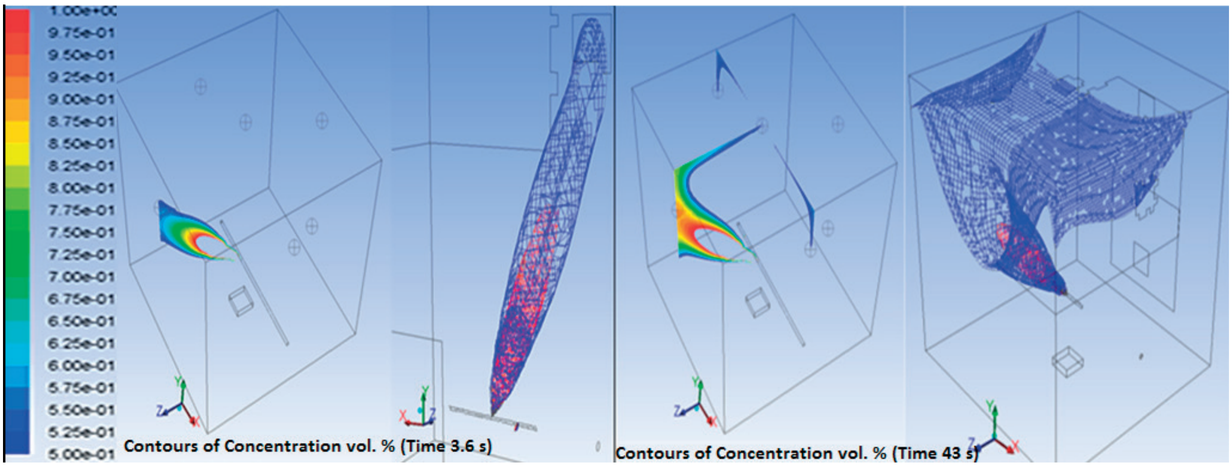

Fig. 8 Local concentrations (0.5 vol. %) during reaction of the sensors Nos. 1 (on the left) and 2, 5 and 6 (on the right)

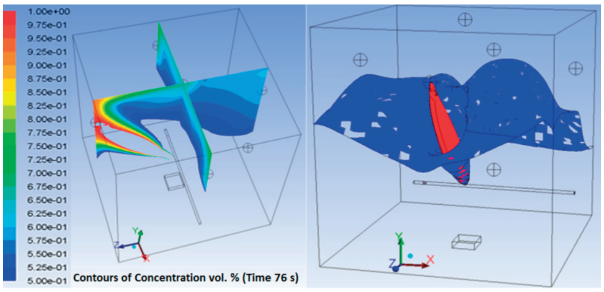

Fig. 10 Local concentrations during reaction of the sensor No. 1 (1 vol. %)

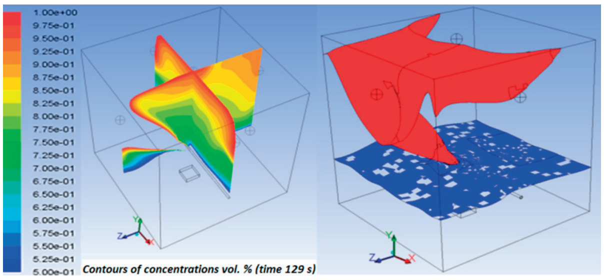

Fig. 11 Local concentrations during reaction of the sensors Nos. 2, 5 and 6 (1 vol. %) [7]

At the time after detection of the sensor No. 3 (0.5% of voluminal concentration) the gas propagated slowly along the rear wall downwards. Large swirl took place in the left part of the vessel (blue bulging on the right side, (Fig. 10). Figure 11 shows location of concentrations during the subsequent reaction of the sensors Nos. 2, 5 and 6 (1% of voluminal concentration). At that time the concentration of 0.5% already settled in one almost horizontal level. Drop of the level of 0.5% was already very slow, unlike the level of 1%.

During detection of the last detector (No. 4) both levels were almost horizontal and they slowly shifted downwards. The right top corner of the image (Fig. 12) shows that concentrations of 0.5% and 1% were created also in proximity of the hole from which the gas leaked, and that they were continuously connected with the levels by bended cones.

At the time of completion of the experiment both levels were under the pipeline which supplied methane (natural gas) into the vessel.

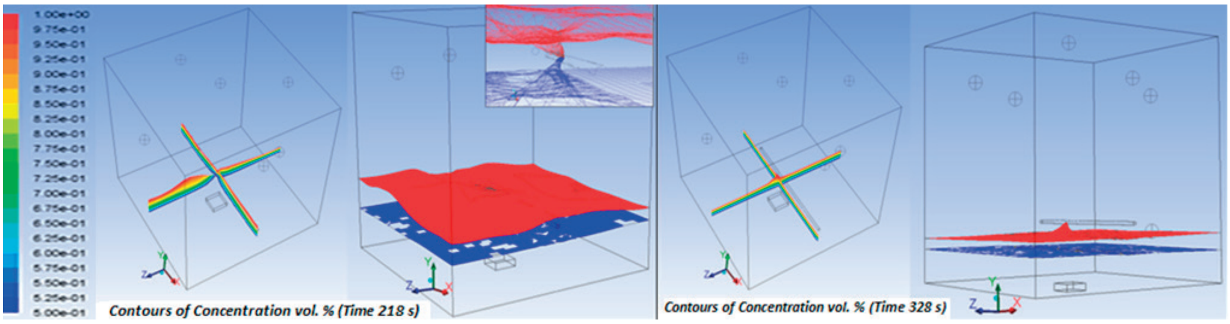

Fig. 12 Local concentrations during reaction of the sensor No. 4 (0.5 and 1 vol. %) [7]

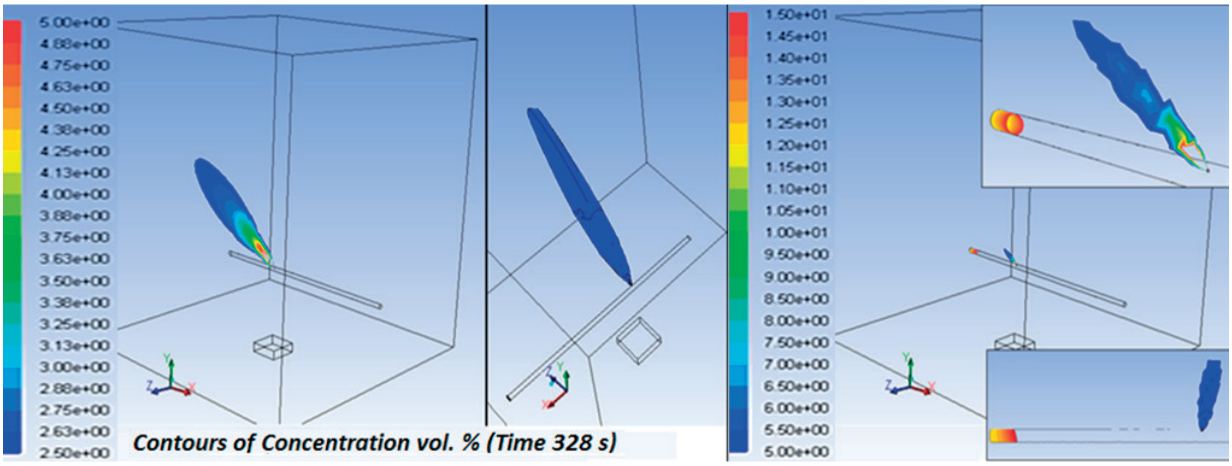

Fig. 13 Dangerous (on the left) and explosive (on the right) concentration right before the end of experiment

6. Formation of dangerous and explosive concentrations at gas escape

The question of safety of experimental measurements was a big issue. The first variant of safeguard consisted in replacement of natural gas by non-inflammable gas. This variant was rejected due to measurement of concentrations at maximum around 20% of the lower limit of explosiveness of natural gas and it was assumed that no explosive concentration should create. The vessel was moreover flushed after each measurement on open air in order to ensure safety during repeated measurements by venting the accumulated gas.

At the end of experiment (reaction of the last sensor) a question arose whether dangerous concentration (50 % of the lower limit of explosiveness) or even explosive concentration of methane was not already created in the measuring vessel, which would make the measurement dangerous for the persons near the vessel. For these reasons we monitored also formation of local dangerous and explosive concentrations. Natural gas is explosive when it reaches concentration of 5 to 15 voluminal percentage [6]. Two spatial levels were created in the program Fluent, which depicted dangerous concentration (2.5 vol. %) and lower limit of explosiveness (5 vol. %). The explosive concentration is moreover depicted in the plane intersecting the axis x. Its location is the same as in the case of evaluation, in chapter 6 ´Propagation of methane in an enclosed space´. Figure 13 shows distribution of contours with dangerous and explosive concentration.

Dangerous concentration was formed only as a paraboloid inclined under the angle of 45°. Figure 13 shows distribution of concentrations within the range of 2.5% to 5% of concentration (from the dangerous concentration to the concentration of the lower limit of explosiveness).

At the moment of termination of the experiment an explosive concentration was formed only in proximity of the leak (hole) from which the gas escaped, and in the pipeline at its blinded end.

7. Conclusions

Borders of local explosive and local dangerous concentrations were determined by mathematical CFD simulation. We obtained moreover a comprehensive image of manner of propagation and increase or decrease of concentrations of natural gas (methane) in the whole area of the given space. Correctness of the mathematical simulation was verified by experimental measurement during which voluminal concentrations of methane were measured at selected points.

So far the propagation of natural gas was investigated only in an enclosed space of simple shape, without internal structuring. Thanks to the good agreement of measurement with the simulation it is possible to move further and to investigate propagation of natural gas in larger spaces with much more complicated internal structure which would better correspond to real buildings or technologies.

The published procedures and results can be used for prediction at real accidents connected with gas leakage in production plants, in households, etc. It is, for example, possible to determine on the basis of numerical simulation the most probable places in which an initiation of explosive concentration could occur and at the same time also to estimate the strength of explosion.

Acknowledgements

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