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MODELING OF GAS EXPANSION IN GARAGES

Abstract: *When changing cars' fuel (hydrogen, methane, oil gas), the demands for safe garages for one car in dwelling buildings are being changed, too. It is necessary to know and understand the expansion of gases in the circumstances of unexpected gas escape to establish the safety rules. With the help of a model garage (1 : 10) we use an experiment to find out the expansion of gases or the concentration on separate measuring points. We measured the concentration of argon, helium and the mixture of hydrogen and argon, methane and argon. We observed the filling and the emptying of the enclosure – model garage. According to the results, we got with the measuring, we searched out suitable mathematical curves, which would well enough list the enlargement of concentration at separate measuring points. We are still looking for a connection between the parameters of the curves, the parameters of measuring and the conditions of the experiments. We will be able to find a suitable safety protection if we know the behaviour of the gases in a concrete closed room.*

Key words: mathematical model, gas expansion, safety in a garage.

INTRODUCTION

Development of new sorts of cars' fuel was caused by anxiety which appeared because of the accumulation of high concentration of carbon dioxide in the atmosphere which is at the same time the result of combustion of carbon dioxides in the fuel. The development of the vehicles has already reached the stage of starting a serial production of the fuel cells driven vehicles with the combustion of hydrogen [8]. Together with the development of new technologies, safety views of using these new sorts of fuel are being developed as well, especially in the field of using hydrogen. The hydrogen driven vehicles present the biggest risk in tunnels and public garages. They present a potential danger in a garage because of possible accidents, which could arise from the hydrogen exhaust. The measure and the co-workers [3] passed a series of tests to study the risk connected to the use of hydrogen technologies in public garages. They had built a building, which had shammed a one-car garage. The test included the ignition of hydrogen, which arose inside the building and researching the effects of deflagration. They analysed the risk of using hydrogen fuel cells. The hydrogen exhaust presents the biggest risk because of the defects in installation [4]. The gas leak appears for various reasons, for example porous material for hydrogen, corrosion in the tank, valve problems, damaged fuel pipe during its work. The leak of hydrogen will be fatal if it happens in a closed room, for example in a lock-up garage or in a parking house. The lower limit of the inflammation of the hydrogen and air mixture can be reach very easily. The worst scenario would be the escape under the pressure directly from a tank.

The practicability of the researches on behaviour of the hydrogen will show up at an occasion of parking a hydrogen driven car in lock-up garages or at installation of fuel cells in closed rooms. Comparing the leak (outlet) of hydrogen, methane and propane (H_2, CH_4 in C_3H_8) Swain [7] tested the exhaust at diffusion, linear and turbulent flow.

Swain et al. [6] tried to explain the moving of hydrogen in closed rooms by using CDF (computational fluid dynamics) modelling. They took the data about helium for the model. Similarly, to this they used helium in the experimental parts of the researches in the study NIST [5]. They tested the effects of helium loose as to the location of its escape from an idealized quarter of the two-car garage. Cariteau et al. [2] handled with distribution of helium, which appears at leak in different locations under a vehicle or in an empty garage. The casing was lessened to a one-car garage, 5.76 m long, 2.96 m wide and 2.42 m high, very well closed, with the measured air change per hour. The total (common) volume of helium 1.09 m^3 was released at a constant speed in the course of time in every experiment, either 105 s or 316 s. It proved that the higher degree of the flow had caused higher concentrations near the ceiling at the end of the release. The vertical profile of the concentrations showed that the distribution of helium is partly stratified (distributed in layers of concentration), with higher degree of the flow, the upper layers are more stratified. The choice of two different horizontal locations in the garage did not have any typical influence on the distribution of helium.

Pitts W.M. et al. [5] described an experiment with helium that serves as a substitute for hydrogen. The experiment was carried out in a garage of a natural size standing next to a dwelling house. They ventilated it physically (naturally) and forcibly. The experiment was carried out in an empty garage and in a garage with a vehicle in it. The garage was prepared for the experiment with helium and was airproof as other typical garages in the USA. The next statement was that helium was still 1.0 m and 1.2 m above the ground after about 2 hours. The measuring showed that the concentration of helium was minimal in an empty garage. About two thirds of helium was lost out of the garage in 4 hours, which means that the highest presence was up to 4 %, that is near the lower limit of flammability for hydrogen / air mixture. They found out that it mixed very lively and behaved in a dispersant.

Gases

When we want to explore the behaviour of a gas in a closed room, we must know their characteristics, specificities and differences first. With suitable knowledge of their characteristics, it would be easier to understand the differences in their expansion in a lock-up garage. We were exploring argon, hydrogen, methane and helium in our research, but in the analyse we decided for argon (the gas is heavier than the air) and helium (which is lighter than air).

Argon is a precious inert gas, colourless and odourless, its serial number is 18 and the atomic mass is 39.95. The atmosphere contains 1% of this gas and is non-flammable. Its relative density is 1.38. The density at 0 °C is 1.78×10^{-3} g/cm^3. Its boiling point is at -186°C, the temperature of melting – point is -189 °C, the critical temperature is -122 °C. Viscosity is 0,022cP (gas). Argon is heavier than air, since it, molar mass is 40 g/mol, as on the other hand the molar mass of air is 29 g/mol. Argon has a similar solubility as oxygen and is 2.5-times more soluble in water than nitrogen. The solubility of argon is 67 mg/l. a high concentration of argon may cause suffocation.

Helium is a precious gas, too, but it has a much lower serial number, that is 2. Its boiling point is at -269 °C and the melting point at -272.2 °C. The critical temperature is -268 °C. It is the second most often found gas on the earth and the second lightest element. It is not poisonous. It is colourless and odourless. Its atomic mass is 4. Helium has many unique characteristics, such as low boiling point, high conductibility and high inertness. The density at 20°C is 0.178×10^{-3} g/cm^3. It is less soluble in water than any other gas; the solubility is 1.5 mg/l. heating the helium may cause an explosion. In case of greater expansion, it is necessary to leave the area. If it is possible, we must prevent the outflow of the gas and the omission of the gas into outflow, sewage - system.

METHODES

Experimental part

We used a model garage in the ratio 1:10 made of 6 mm thick polycarbonate for testing the gas expansion. The model garage is made of casing of the model, a coil, an air pipe valve, a gas-pipe valve, the switch-on connection to the battery (accumulator), three measuring points with a capillary and a ventilation opening. Glass capillary for in taking the measured gas were 200 microns thick. The length of a capillary was at measuring at an upper measuring point 4.5 cm and at measuring at a lower measuring point 24 cm. the ventilation opening is meant for ventilation of the model garage. The capillary is there to perceive parts in the model. The coil was not used in our experiment but was meant for loading (charging) the ignition plug, which could be used as a source of ignition power for explosions. The air-pipe valve was not used in our experiment either, but it can be used for ventilation. The gas-pipe switch-on is meant for leading the gas into the model garage. The model is 60 cm long, 25 cm high, 30 cm wide, and the diameter of the opening is 12 cm. there is a ventilation opening on the right. During the measuring, it was closed with foil so that the gas could not leak out of the chamber.

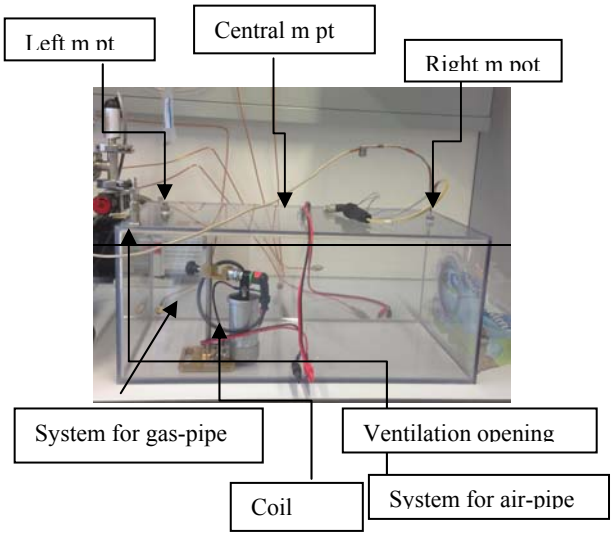

Figure 1. *The photo of the model garage (Source [1])*

We used the following gases and the gas mixtures in the given concentration from Linde supplier:

Table 1. *The review of gases with concentration (Source [1])*

No	Gas	The quality gas mark	Gas concentration (%)
1	Argon (Ar)	Argon 5.0	Ar - 100
2	Argon - methane (Ar - CH_4)	Argon 5.0, Methane 4.5	Ar – 95, CH_4 - 5
3	Argon – hydrogen (Ar - H_2)	Argon 5.0, Hydrogen 4.5	Ar – 95, H_2 - 5
4	Argon – oxygen (Ar - O_2)	Argon 5.0, Oxygen 4.5	Ar – 95, O_2 - 5
5	Helium (He)	Helium4.5	He - 100

In the experimental part we used mass spectrometer, type QMG 220 F1, mark Pfeiffer Vacuum, PrismaPlusTH. The picture below shows a mass spectrometer which is used to define molecular structure.

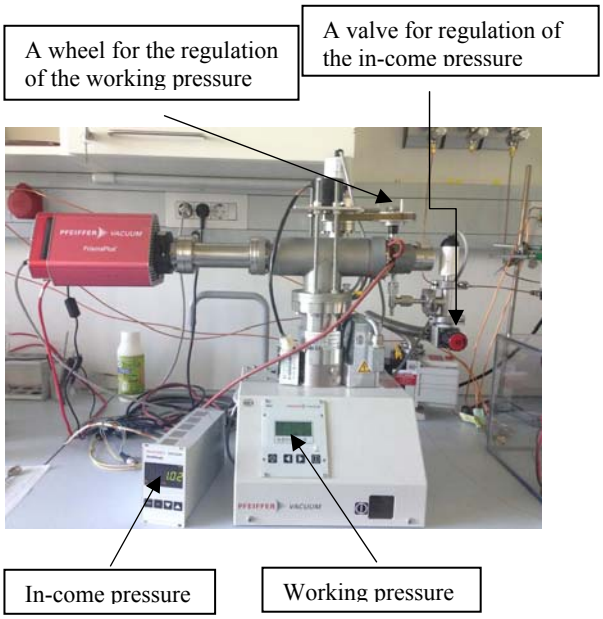

Figure 2. *Mass spectometer(Source [1])*

The mass structure of the gas at a measuring point we expressed with the molecular mass of the measured gas or gases. We measure at the constant working pressure of the mass spectrometer, as we set it up before the impetus of the computer programme for noting down the results 2.5 x 10^{-6} mbar. The in-come pressure was set up to 1.01 mbar with the valve for regulation of the pressure before the measuring. We read the data of the changing from the programme QUADERA, taking the data every 20 milliseconds. The gas was supplied with a flow 10 ml/min and with a flow of 100 ml/min. The room temperature was about 22 ºC, the humidity of the room was between 30 % and 40 %.

We were carrying out the measuring with gases: Ar, Ar-CH_4, Ar-H_2, He. We chose helium as a light gas (100% concentration), and argon as a heavy gas (95% concentration) and two mixtures of argon with hydrogen (5% concentration) and methane (5% concentration). We were using the mixtures with argon because of the flammability and the ability of explosion of the gases. Helium was chosen as the second lightest gas on the earth, just next to the hydrogen, and because it can be a good approximation to the behaviour of hydrogen. We measured with two different flows, 10 ml/min and 100 ml/min.

The measuring was carried out for every gas or gas mixture at six measuring points:

- left, central and right upper measuring point,
- left, central and right lower measuring point.

The measuring conditions were the same at every measuring:

- the working pressure was set up to 2.5 x 10^{-6} mbar,
- the in-come pressure to 1.01 mbar,
- the gas was supplied at a flow of 10 ml/min and 100 ml/min,
- we read the data of changing from the programme QUADERA,
- the data were taken every 20 milliseconds,
- the temperature of the room was about 22 ºC,
- the humidity of the room was about 30 % and 40 %.

Carrying out the computer shams

Using a computer sham programme we present a situation from the real world. We carried out four computer shams, argon with coil, argon a smaller vehicle, helium with a coil, helium with a smaller vehicle. In these cases, we used green colour for argon and helium small parts. We performed a sham of a 5-minute in blowing of the gas under the same conditions as we had had in the experimental part. At CFD (Computational Fluid Dynamics) modelling, there are three programme moduli included into the programme scheme (design). The first programme modulus is a modulus, which contains a model for geometry generalizing. The second one contains numerical sham, and includes border and starting conditions. The third modulus is an after-process modulus that shows the results of sham. It is called Smoke view and is used for visualisation and manipulation of the results gained from the second model.

Mathematical modelling

According to the gained results of measuring the concentration of gases at separate measuring points, we tried to find suitable mathematical curves, which are, well enough in accordance with the results of measuring. We tried to find the curves, which are connected to only three measuring points.

THE RESULTS

Argon

The in blowing of the argon began approximately after 2 minutes. In the picture below the results show that argon started growing up by jerks at the measuring point down on the ground (stronger at the point of in-blowing, and slower at the points further away), later on the rise calmed down and became almost linear. At the beginning of the in blowing, the changes are quick; moving is obviously turbulent and depended on the distance of the source. Already after 5 minutes, constant differences between separate measuring points are restored, the rise is almost linear. The time of measuring of the left and the central measuring point is 31 minutes, and of the right one about 30 minutes.

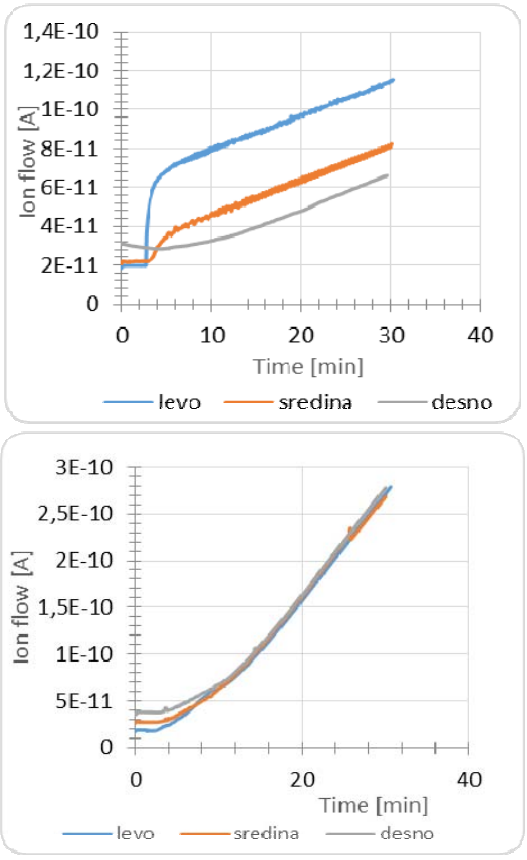

Figure 3. *Comparison of the amount of argon at the lower and upper measuring points (the flow is 100 ml/min), (levo – left, sredina – middle, desno – right). Source [1]*

The following measurements with argon were done at 10-times smaller flow. At lower measuring points, we are establishing that the rise of the ion amount is similar to the exponent function. At bigger in-put of the molecules, the exponent function of rise is < 1, and at small in-put the exponent is >1. At the right measuring point, the rise is too small, and that is why the form of the curve is being changed. The time of measuring at the central measuring point is 30 minutes.

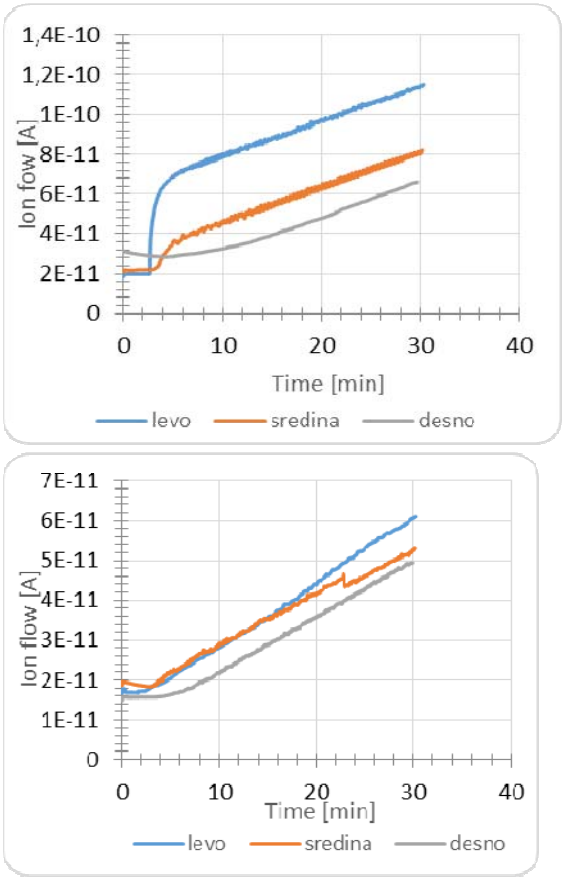

Figure 4. *Comparison of the amount of argon at the lower and upper measuring points (the flow is 10 ml/min), (levo – left, sredina – middle, desno – right). Source [1]*

The graph of the final distribution of argon shows that the concentration at lower and upper measurements are of the greatest difference when the flow of the gas is bigger, where the total amount of the in-blown gas is 3000 ml (0,0979 kg).

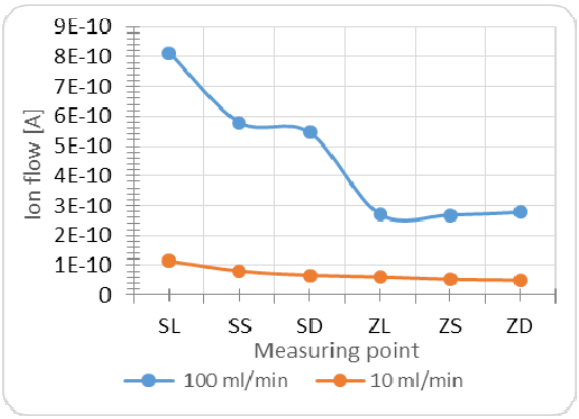

Figure 5. *Comparison of ion flow of argon at measuring points after 30min. (LD–left down, CD–central down, RD-right down, LU–left up, CU–central up, RU-right up) Source [1]*

Helium

Helium [He] is with the serial number 2, the second lightest element in the periodic system. Since helium is not flammable and it is the second lightest element (next to the hydrogen) in the periodic system, it seemed to us as the most suitable gas, which could bring us at least a little closer to hydrogen.

The in blowing started after 2 minutes. The pressure of the valve was 2 bars. Helium with the flow of 10 ml/min at the upper measuring points started growing up by jerks (stronger at the point of in blowing and slower at the points further away). The rising continued as a straight line. The time of measuring at the left, central and right measuring points is about 29 min.

The gas behaved similarly at the lower measuring points, too, but only with a half of the amount. Only near the point of in blowing the amount of helium was similar to the one under the ceiling all the time.

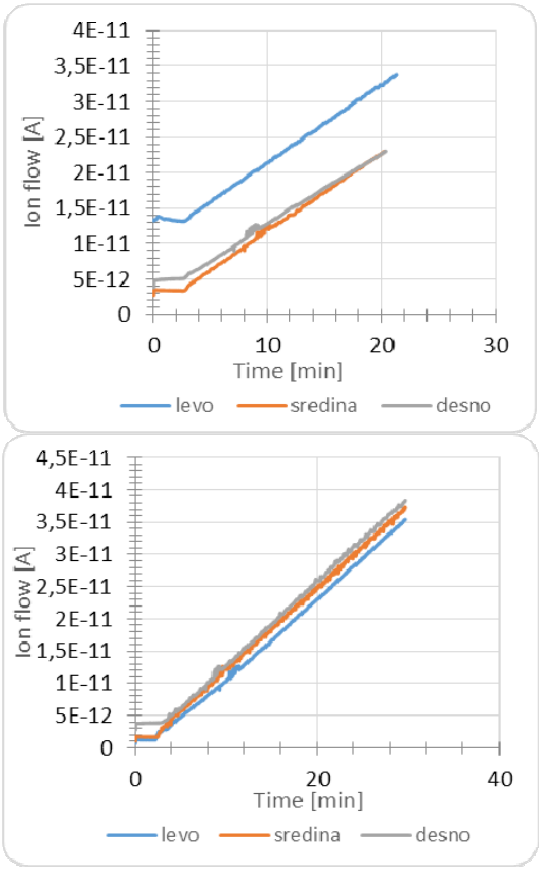

Figure 6. *Comparison of the amount of helium at the lower and upper measuring points (the flow is 10 ml/min), (levo – left, sredina – middle, desno – right). Source [1]*

The in blowing started after about 2 minutes. The ion flow was at the upper measuring points similar to case with a weaker in blowing, but with a 6.5-times bigger amount (quantity). At the lower measuring points, it is 10-times bigger. The time at every measuring point is about 30 minutes.

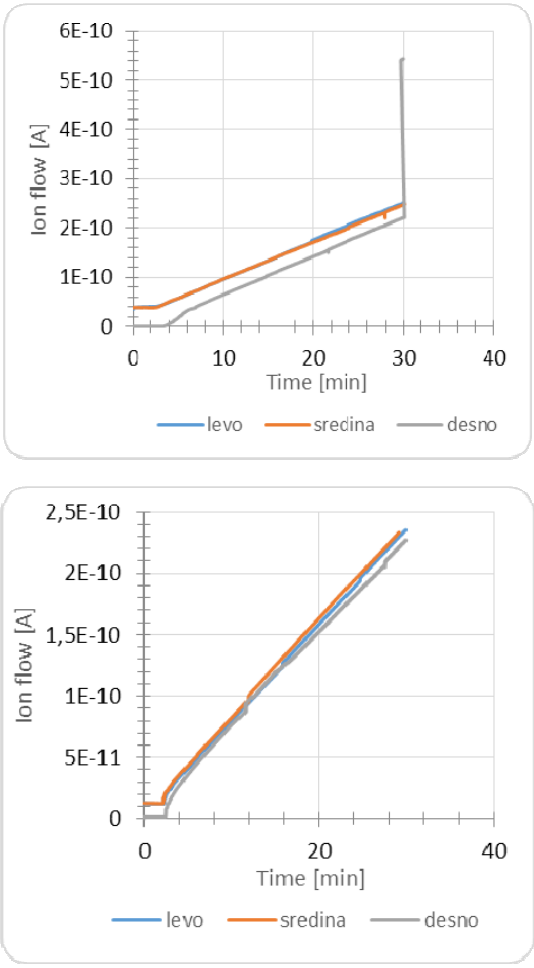

Figure 7. *Comparison of the amount of helium at the lower and upper measuring points (the flow is 100 ml/min), (levo – left, sredina – middle, desno – right). Source [1]*

The graph of the comparison shows the concentration at lower and upper measurements. The different between both of them is not as obvious as it was with previous comparisons where the biggest flow dominates strongly. The biggest flow still presents the greatest oscillation, namely at the right lower measuring point which is probably the consequence of the distant source of the in blowing.

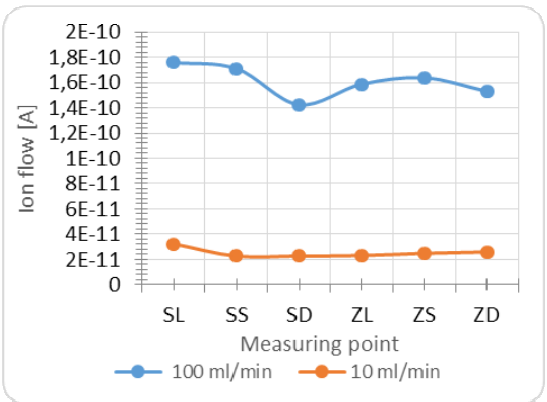

Figure 8. *Comparison of ion flow of helium at measuring points after 30min. (LD–left down, CD–central down, RD-right down, LU–left up, CU–central up, RU-right up) Source [1]*

Computer sham

The computer sham shows the state that argon spreads on the ground of the observed room. When the small parts come to an obstacle, for example the walls of the room or a specific obstacle like a coil, they start to thicken and at the same time, whirling or turbulent flow arises. It was found out that the argon parts move faster with the computer model with argon and a coil than with a computer model of a garage with a car because the parts there ran into obstacle and that caused more turbulent moving (at least the model shows so).

Helium spreads on the upper half of the room. When the parts start gathering and occupy the upper part of the model garage, the parts start turbulent whirling. They slowly occupy the model garage by this gathering (they supplant the air). The sham shows that the coil does not present an obstacle for the parts. We can as well confirm the hypothesis that the parts of helium were kept in the upper part of the model garage.

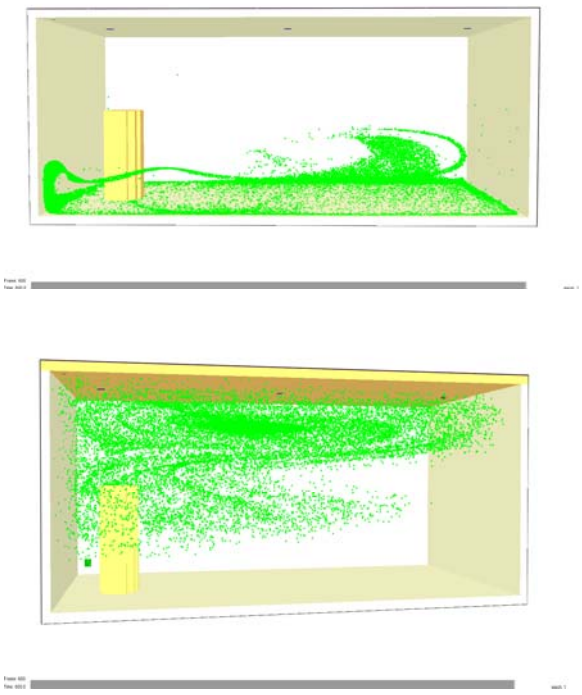

Figure 9. *Comparison of the models of outlet of argon and helium after 10 min with the flow 100 ml/min. Source [1]*

Mathematical model

We are looking for functional connection between ion flow and the time of the outlet of the gas at a definite measuring point. The results of the measuring show that the growth of concentration is connected to exponent function. If we write down the concentration (the number of ions at a measuring point) with a variable y and the time with a variable t, we can write down the expected equation:

$$y = \alpha(t - t_1)^{\beta} + y_1 \quad (1)$$

α and β are the unknown parameters in the equation. We fill in the equation (1) the values from the beginning of the measuring (t_1 , y_1), at half of the measuring ($t_{n/2}$, $y_{n/2}$) and at the end of the measuring (t_n , y_n).

$$y_{n/2} = \alpha(t_{n/2} - t_1)^{\beta} + y_1 \quad (2)$$

$$y_n = \alpha(t_n - t_1)^{\beta} + y_1 \quad (3)$$

We solve the system of the equations (2) and (3), and we get the parameters of the equation:

$$\alpha = \frac{y_n - y_1}{(t_n - t_1)^{\beta}} \quad (4)$$

and

$$\beta = \frac{ln\left(\frac{y_{n/2} - y_1}{y_n - y_1}\right)}{ln\left(\frac{t_{n/2} - t_1}{t_n - t_1}\right)} \quad (5)$$

The legend of the equations:

t_1 = the initial time (when we start in-blowing),

t = time as an variable,

$t_{n/2}$ = time at a half of the measuring,

t_n = time at the end of measuring,

y_1 = the initial number of ions at a measuring point,

y = the number of ions at a measuring point as an variable,

$y_{n/2}$ = the value of the number of ions at a measuring point at a half of the measuring at a measuring point,

y_n = the number of ions at a measuring point at the end of measuring.

The comparisons of the measured and calculated results show great similarity in the results. Let us look at a comparison and calculation for argon 100 ml/min right down.

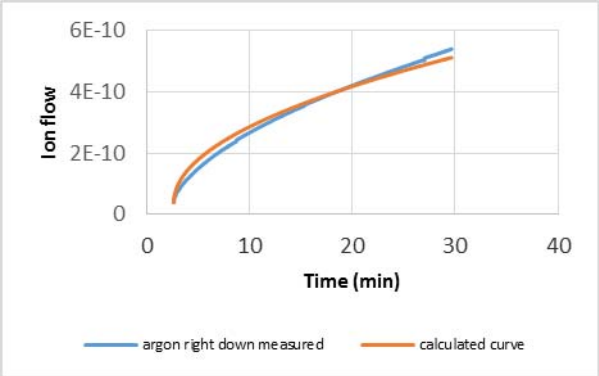

Figure 10: *Comparison of the measurements (blue) and the calculated (red) curve for argon 100 ml/min at the measuring point right down.(My own source)*

In the model, we use the function:

$$y = 6{,}8 \cdot 10^{-11}(t - 2{,}63)^{4{,}61} + 3{,}95 \cdot 10^{-11} \quad (6)$$

We found out that an average absolute difference between the measured and the calculated value is:

$\Delta = 7{,}6 \cdot 10^{-12}$

and the relative fault: $0{,}021$. The standard deviation (declination) of the difference is $5{,}2 \cdot 10^{-11}$.

We get similar results for helium 100 ml/min at a lower and upper measuring point on the right.

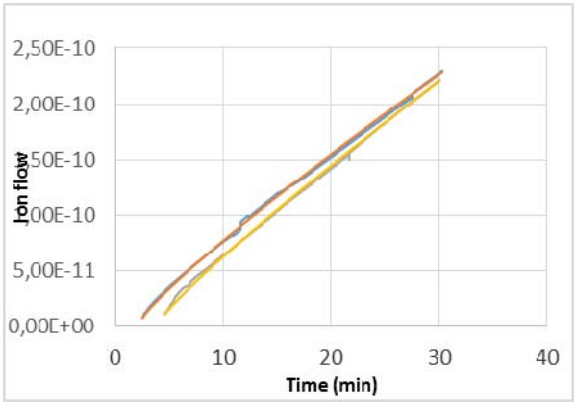

Figure 11: *Comparison of the measurements and the calculated curve for helium 100 ml/min at measuring points up and down on the right. (Blue – measurement up, red – calculated up, grey – measurement down, orange – calculated down). (My own source)*

Above we used the function:

$$y - 1{,}2 \cdot 10^{-11}(t - 4{,}35)^{0{,}88} + 3 \cdot 10^{-11} \quad (7)$$

An average difference between the measured and the calculated results is $1.7 \cdot 10^{-12}$, the standard deviation is $9.8 \cdot 10^{-13}$and the relative difference of the averages is$1{,}39 \cdot 10^{-2}$.

For the lower measuring point, we used the function:

$$y = 1{,}02 \cdot 10^{-11}(t - 4{,}39)^{0{,}93} + 9{,}12 \cdot 10^{-12} \quad (8)$$

An average difference between the measured and the calculated results is $1{,}5 \cdot 10^{-12}$, the standard deviation is $1{,}3 \cdot 10^{-12}$ and the relative difference of the averages is $1{,}29 \cdot 10^{-2}$.

The next step will be looking for the connection between the parameters of measuring and the parameters of function. (How do α and β depend on the amount of the in-blown gas and on the position of a measuring point, and maybe as well on the geometry of a room, etc.)

DISCUSSION

The results of the measuring of the concentration of the unexpected outlet of the gas gave the expected measures. For the continuous growth of concentration the initial external conditions that do not change, are important. Every change (for example the pressure of the measuring instrument) caused discontinuous changes of concentration. The speed of the gas outlet is very important for the growth of the concentration. At fast outlets the amount of concentration at separate measuring points grow with an exponent function, the exponent of which is bigger than 1. In some cases, we can even get a linear rise, usually somehow away from the outlet point. The results agree with the results received by Montevalli et al [4] with the experiment of different outlets of hydrogen from the tank.

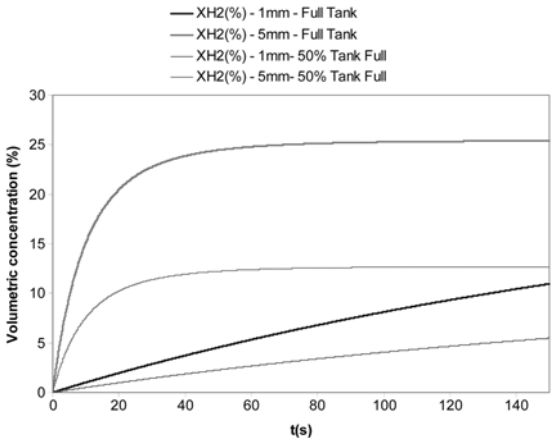

Figure 12: *Outlets at different amounts of hydrogen in the tank. Source: Montevalli et al [4]*

The forms of the curves confirm our upper consideration and the similarity with our mathematical model. Our research found out how different gases behave at an outlet in a lock-up room – garage. For more precise explanation of the connections of growth of the concentration with the time it would be necessary to study the moving of the molecules and the growth of the pressure in a room. Measurements gave us indicators of the directions of the research, they also confirmed the results of some preceding measurements, and they enable better understanding.

CONCLUSION

We carried out the measuring and the computer shams to find out the moving of the gases in a garage at an unexpected outlet. They show that heavier gases in a garage at an unexpected outlet. They show that heavier gases spread on the ground of a model garage and they fill in the room from the ground upwards, lighter gases, on the other hand, are kept under the ceiling of a model garage and fill in the room from the ceiling downwards. The speed of gas gathering under the ceiling depends on the lifting force. That is why we had difficulties in reaching the explosive mixture on the ground if the outlets of hydrogen were low. Of course, we could easily reach it under the ceiling, what can be seen from our measurements. However, the time diagrams show that the gas fills in the whole room. It would be possible to reach critical concentrations on the ground, too, at a big enough and longer outlet. At a smaller flow and an obstacle, as presented by a coil in the model, we found out that despite the smaller flow the turbulences are bigger. The differences between upper and lower measuring points are better defined at greater flows, that means that the characteristics of a gas more outstandingly affect the expansion at greater flows. It is true for every experimental measurement we carried out that the further away from the source we are the smaller are the differences between the concentrations at the bottom and the concentrations under the ceiling. The differences grow if the flow grows. All the computer shams show that the obstacles cause better-defined turbulent move of the gas, and consequently bigger declinations from the linear rise of the amount of the gas at separate measuring points. The bigger obstacles lessen the speed of moving molecules in a direction; obviously, they lose kinetic energy gained at an outlet.

We can infer from the measurements and the computer shams, how we could effectively equip a model garage with suitable sensors and ventilation. When the gases are heavier than the air (oil gases, petrol vapours) the sensors would be installed onto the ground of the model garage. We would as well install the sucking-out on the ground or in the ground of the garage. When we use lighter gases (hydrogen, helium) the sensors should be on the ceiling of the model garage, and the sucking-out or just the ventilation would be installed at the ceiling of the garage. This would enable us to reduce the risk of an explosion, as we could prevent from critical concentrations of gases right where they gather the fastest. As the literature suggest, it would be necessary to prevent the gathering of gas in the car in separate car "pockets" (hood, boot, passengers' cabin). That might be prevented by suitable openings on the car. It would make sense to additionally looking for the dependence of the parameters of the equation (1) from the initial and external parameters, such as the speed of the outlet, the distance from the outlet point, the kind of gas, the geometry of the obstacles etc.

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Jože Šrekl was university teacher in the Technical Safety Section of the Faculty of Chemistry and Chemistry Technology, University in Ljubljana. He graduated from the Science and Technology Faculty, Section for Mathematics. He received Master degree at Zagrebačko sveučilište (Zagreb University), Prirodoslovno matematički fakultet (Science-mathematical Faculty and he was graduated from the Faculty of Chemistry and Chemistry Technology, University in Ljubljana, with the Ph.D. degree in chemical technology. There he was busy with applications of statistical methods of security and fire safety. He co-operated in two international researches, financed by the project, and two researches, financed by the Ministry of Defence of the Republic Slovenia. He published five important science articles in the world magazines as the first author; he co-worked in three bigger international conferences and many conferences with international participation. He is an author of some university textbooks and a reviewer (critic) of some textbooks, monographies and articles, published in international magazines. He is retired from 1st October 2015.

MODELIRANJE ŠIRENJA GASA U GARAŽI

Jože Šrekl

Rezime: *Zamenom goriva za automobile (vodonik, metan, LPG) menjaju se uslovi bezbednosti garaže u sklopu stambenog objekta. Za uspostavljanje principa bezbednosti treba poznavati i razumeti širenje gasova koji se neočekivano oslobađaju. Eksperimentalno ispitivanje modela garaže (1:10) ukazuje na širenje određenih gasova ili koncentracije na pojedinim mernim mestima. Merili smo koncentracije argona, helijum i smeše vodonika sa argonom, metanom, argonom. Posmatrali smo punjenje i pražnjenje komore - modela garaže. Na osnovu izmerenih rezultata, utvrdili smo matematički krivu koja dobro opisuje povećanje koncentracije na pojedinim mernim mestima. U potrazi smo za daljim povezivanjem parametara krive i parametara mernih tačaka u uslovima eksperimenata. Saznanja o ponašanju gasova u konkretnom zatvorenom prostoru omogućavanju upravljanje rizikom odnosno kreiranje odgovarajuće zaštite od opasnosti.*

Ključne reči: matematički model, širenje gasa, sigurnost u garaži.