PASSIVE VENTILATION OF A SUSTAINED GASEOUS RELEASE IN AN ENCLOSURE WITH ONE VENT

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ABSTRACT

A model for prediction of steady-state uniform concentration of a sustained gaseous leak in an enclosure with passive ventilation through one vent is described. Theoretically natural ventilation models under-predict up to twice lower concentrations of releasing gas and over-predict up to twice higher concentrations compared to the model of passive ventilation. The distinctive feature of passive ventilation is positioning of the neutral plane anywhere below the half of the vent height whereas it is located at about half vent height in the case of natural ventilation. The model is compared against experimental data on uniform and non-uniform distribution of helium concentration in the enclosure with one vent of different size and various release flow rates. The model predictions of observed in the experiments maximum concentrations of helium with the conservative discharge coefficient value C_D=0.60 (the best fit range is from 0.60 to 0.95) are closer to measured data than calculation by a model based on the natural ventilation assumptions even with "tuned" C_D=0.25. The engineering nomogram to calculate a release mass flow rate leading to 100% concentration of gas in an enclosure as a function of vent width and height is presented. The equation behind the nomogram is verified by CFD simulations and the appropriate discharge coefficient is derived for use in the equation as C_D=0.85. Effectiveness of different vent configurations is compared based of the ventilation parameter $A\sqrt{H}$. A new criterion for mixture uniformity in a ventilated enclosure is suggested and applied to available experimental data. It is concluded that the maximum and minimum mole fractions deviate from the average mole fraction by no more than 20% when the criterion is above 4.

NOMENCLATURE

A	area (m^2)
B	varaible (-)
C	concentration (% by volume)
C_D	discharge coefficient (-)
D	nozzle diameter (m)
g	gravity acceleration (m/s^2)
g'	reduced gravity (m/s^2)
H	vent height (m)
h	height above enclosure floor (m)
h_1	distance from floor to vent bottom edge (m)
h_2	distance from floor to vent top edge (m)
K_1	constant (0.282)
L	jet length (m)
M	molecular mass (kg/kmol)
M_0	momentum flux (Pa)
MF	mass fraction (-)
$\dot{m}$	mass flow rate (kg/s)
p	pressure (Pa)
Q	volumetric flow rate through vent (m^3/s)
Q_0	volumetric flow rate of gas leak (m^3/s)
R	universal gas constant, *8314.4* J/K/kmol
Ri	Richardson number (-)
T	temperature (K)
U	velocity (m/s)
UC	uniformity criterion (-)
V	enclosure volume (m^3)
W	vent width (m)
w	distance along the vent (m)
X	volumetric fraction (-)
x	jet length from a release source (m)
Greek	
α	constant
ρ	density (kg/m^3)
Subscripts	
a	air
ent	entrainment
ext	external
g	gas
H2	hydrogen
int	internal

mix	mixture	*NP*	neutral plane
N	nozzle		

1.0 INTRODUCTION

Unignited release of flammable gas in an enclosure is a typical scenario of incident/accident that could lead to loss of life and property if not dealt with professionally. Unfortunately, there is a lack of understanding of underlying physical phenomena and absence of thoroughly validated tools for safety engineering. For example, correct prediction of steady-state concentration of a sustained leak of hydrogen in an enclosure with one vent is not currently possible in a wide range of realistic accident scenarios as will be demonstrated in this study. How the sustained leak mass flow rate and vent parameters are related to predict that the enclosure will ultimately be filled in by 100% of flammable gas? To answer these and other questions relevant to safety of indoor release of hydrogen, this study aims to develop and validate a model for passive ventilation of a sustained release of hydrogen, i.e. the leak with arbitrary but constant flow rate, in an enclosure with one vent.

In 1962 Brown and Solvanson [1] suggested that the volumetric flow rate, Q, through a half of a single rectangular vent of area, A, and height, H, during natural ventilation of air in a building is

$$Q = \frac{1}{3} C_D A \sqrt{g' H} \,, \tag{1}$$

where $g' = g(\Delta\rho/\bar{\rho})$ is the reduced gravity in which g is the acceleration of gravity, $\Delta\rho = (\rho_{ext} - \rho_{int})$ is the density difference, $\bar{\rho} = (\rho_{ext} + \rho_{int})/2$ is the average density, and ρ_{ext} and ρ_{int} are the densities of the fluid remote from the wall outside and inside the enclosure respectively. The assumption used for derivation of this equation for natural ventilation of air is the equality between volumetric flow rate of air entering and leaving enclosure through the vent. This implies that only half of the vent area is occupied by gases flowing out. This is a typical approximation for natural ventilation of air under normal conditions of building operation. However, this is definitely not applicable for comparatively large unscheduled release of flammable gas, e.g. from hydrogen or fuel cell system, when at flow rates above a certain limit the whole vent area can be occupied by flowing out hydrogen.

In 1999 Linden [2] dropped 1/3 in Eq. 1 that generated future uncertainties in the selection of value of the discharge coefficient C_D by other researchers (three times smaller values of C_D can be expected just to compensate the drop of the coefficient 1/3). Cariteau and Tkatschenko [3] rewrote the equation without 1/3 in terms of the volumetric fraction of hydrogen in air, X, to carry out the comparison with their experiments on helium release in an enclosure with one vent, as

$$X = \left[\frac{Q_0}{C_D A (g' H)^{1/2}} \right]^{2/3} , \tag{2}$$

where Q_0 is the volumetric flow rate of release, and the reduced gravity is $g' = g(\rho_{air} - \rho_{H2})/\rho_{air}$. The accuracy of Eq. 2 [3] for natural ventilation to predict gas concentration will be compared in this study against derived here an exact solution for gas concentration in conditions of passive ventilation.

2.0 MODEL FOR UNIFORM HYDROGEN CONCENTRATION

2.1 Mathematical Model

The neutral plane (NP) is a horizontal plane where pressure inside and outside an enclosure are equal. In general case of passive ventilation of the enclosure with release of gas lighter than air, the neutral plane is located at or below the half height of the vent for steady-state conditions. Below NP air enters the enclosure and above NP lighter hydrogen-air mixture exits the enclosure (Fig. 1, left).

The pressure inside and outside the enclosure follows the hydrostatic equation and can be written as $P_{int}(h) = P_{NP} - \rho_{mix} g(h - h_{NP})$ and $P_{ext}(h) = P_{NP} - \rho_{air} g(h - h_{NP})$ respectively. Thus, the pressure difference at the vent as a function of height is $\Delta P(h) = (\rho_{air} - \rho_{mix}) g(h - h_{NP})$. The velocities of flowing out mixture and flowing in air are, following the Bernoulli's equation, $U_{mix}(h) = \sqrt{2g(\rho_{air} - \rho_{mix})(h - h_{NP})/\rho_{mix}}$ and $U_{air}(h) = \sqrt{2g(\rho_{air} - \rho_{mix})(h_{NP} - h)/\rho_{air}}$ respectively. Mass flow rate of hydrogen-air mixture outflow and air inflow through the vent can be obtained by integration of mass flow rate above and below NP respectively

$$\dot{m}_{mix} = W \cdot \int_{h_{NP}}^{h_2} \rho_{mix} dh \cdot U_{mix}(h) = W \cdot (h_2 - h_{NP})^{3/2} \frac{2}{3} \sqrt{2\rho_{mix} g(\rho_{air} - \rho_{mix})}\,, \tag{3}$$

$$\dot{m}_{air} = W \cdot \int_{h_1}^{h_{NP}} \rho_{air} dh \cdot U_{air}(h) = W \cdot (h_{NP} - h_1)^{3/2} \frac{2}{3} \sqrt{2\rho_{air} g(\rho_{air} - \rho_{mix})}\,. \tag{4}$$

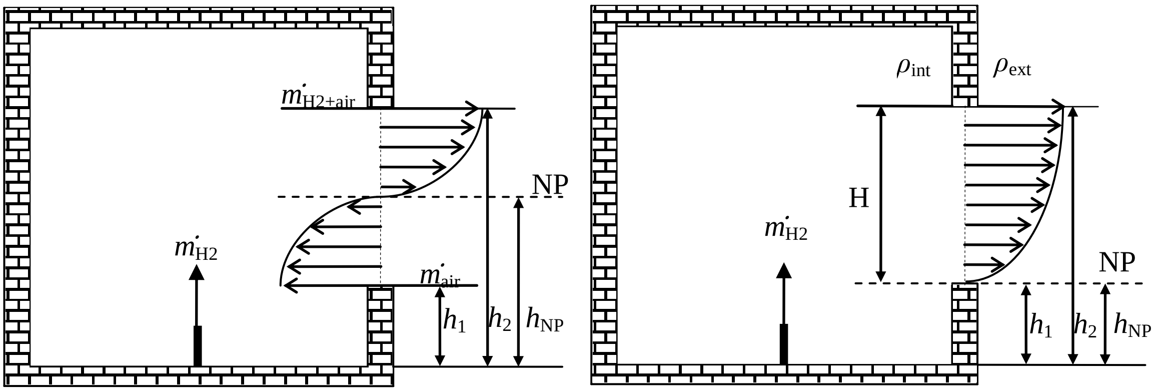


Figure 1. Flow velocity through the vent for a case when neutral plane is between the lower edge and half height of the vent (left), and for the case when neutral plane is at the lower edge of the vent (right)

The mass flow rate of hydrogen-air mixture flowing out of the enclosure is equal to the mass flow rate of air flowing into the enclosure through the vent plus the mass flow rate of the hydrogen entering the enclosure from the release source, i.e. $\dot{m}_{mix} = \dot{m}_{air} + \dot{m}_{H2}$, for the steady-state conditions. Thus, the hydrogen mass flow rate can be obtained by subtraction Eq. 4 from Eq. 3, i.e. $\dot{m}_{H2} = \dot{m}_{mix} - \dot{m}_{air}$,

$$\dot{m}_{H_2} = \frac{2}{3} W \sqrt{2g(\rho_{air} - \rho_{mix})} \left(\sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2} - \sqrt{\rho_{air}} (h_{NP} - h_1)^{3/2} \right). \tag{5}$$

The hydrogen mass flow rate can be also calculated by the integration of mass fraction of hydrogen in the mixture flowing out through the upper part of the vent as

$$\dot{m}_{H_2} = W \cdot \int_{h_{NP}}^{h_2} MF_{H_2} \rho_{mix} U(h) dh = \frac{2}{3} W \sqrt{2g(\rho_{air} - \rho_{mix})} \cdot MF_{H_2} \cdot \sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2}. \tag{6}$$

Equating (5) and (6) gives

$$\sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2} - \sqrt{\rho_{air}} (h_{NP} - h_1)^{3/2} = MF_{H_2} \cdot \sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2} \tag{7}$$

or

$$B = \frac{h_{NP} - h_1}{h_2 - h_{NP}}\,, \tag{8}$$

where for shortness B denotes

$$B = \left(1 - MF_{H_2}\right)^{2/3} \left(\frac{\rho_{mix}}{\rho_{air}}\right)^{1/3} . \tag{9}$$

From Eq. 8 a height of the neutral plane can be calculated as

$$h_{NP} = \frac{h_1 + Bh_2}{1 + B} . \tag{10}$$

The mass flow rate of hydrogen in the hydrogen-air mixture flowing out of the vent is equal to the mass flow rate of hydrogen in the release source. Hence, Eq. 6 can be rewritten as

$$Q_0 \cdot \rho_{H_2} = \frac{2}{3} W \sqrt{2g(\rho_{air} - \rho_{mix})} \cdot MF_{H_2} \cdot \sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2} . \tag{11}$$

Let us rewrite Eq. 11 in the form close to Eq. 2 to compare Eq. 2 derived in the assumptions of natural ventilation of air in a building with Eq. 11 derived for the passive ventilation of hydrogen in an enclosure with one vent. Firstly, from Eq. 10 bearing in mind that the vent height $H=h_2-h_1$ the following can be rearranged

$$h_2 - h_{NP} = h_2 - \frac{h_1 + Bh_2}{1 + B} = \frac{h_2 + Bh_2 - h_1 - Bh_2}{1 + B} = \frac{h_2 - h_1}{1 + B} = \frac{H}{1 + B} . \tag{12}$$

The equation for volumetric fraction of hydrogen in the enclosure is (its validity can be easily demonstrated by substitution of a hydrogen volumetric fraction, $X=V_{H2}/(V_{H2}+V_{air})$, into this equation and multiplying nominators and denominators on left and right hand sides of the equation)

$$X = \frac{\rho_{air} - \rho_{mix}}{\rho_{air} - \rho_{H_2}} , \tag{13}$$

and thus

$$\frac{\rho_{mix}}{\rho_{air}} = 1 - X\left(1 - \frac{\rho_{H_2}}{\rho_{air}}\right). \tag{14}$$

Mass fraction and volumetric fraction of hydrogen are related by definition through the equation

$$MF_{H_2} = \frac{X\rho_{H_2}}{\rho_{mix}} . \tag{15}$$

Finally, Eq. 11 for passive ventilation can be written in the following form convenient for comparison with Eq. 2 for natural ventilation of air in a building (after the introduction of the discharge coefficient, C_D, as a multiplier to the vent area, A)

$$X = f(X) \cdot \left[\frac{Q_0}{C_D A (g' H)^{1/2}}\right]^{2/3} , \tag{16}$$

where function $f(X)$, which defines the difference between the approximate solution for volumetric fraction of hydrogen by natural ventilation Eq. 2 and the exact solution of the problem by passive ventilation theory presented here (Eq. 16), is

$$f(X)=\left(\frac{9}{8}\right)^{1/3}\cdot\left\{\left[1-X\left(1-\frac{\rho_{H_2}}{\rho_{air}}\right)\right]^{1/3}+(1-X)^{2/3}\right\}. \tag{17}$$

It is worth noting that Eq. 16 is derived in the assumption of mixture uniformity within the enclosure.

2.2 Comparison of Predictive Capability of Equations for Passive and Natural Ventilation

Function $f(X)$ gives the deviation of the exact solution of the problem within the assumptions, i.e. Eq. 16 for passive ventilation, from the approximate solution for unscheduled release of gas, i.e. Eq. 2 for natural ventilation of air in buildings. Figure 2 (left) shows the change of $f(X)$ with hydrogen volumetric fraction in air (solid line) compared to $f(X)$=1 for natural ventilation (dash line).

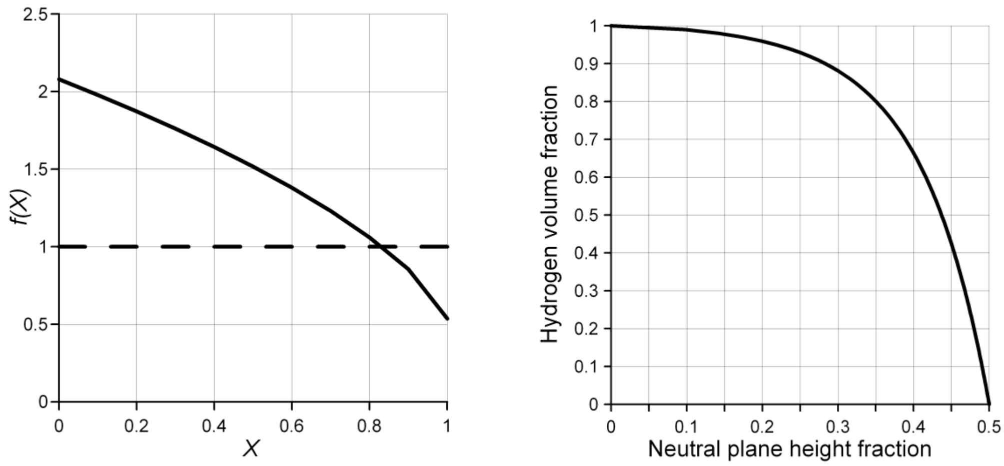


Figure 2. Left: function $f(X)$ for passive ventilation (solid line) and for natural ventilation (dash line). Right: hydrogen volume fraction in enclosure as a function of neutral plane height fraction

Figure 2 (left) demonstrates that $f(X)$ can be twice more than 1 for small volumetric fractions of hydrogen and twice less than 1 for very high volumetric fractions. This means that hydrogen concentrations predicted by Eq. 2 for natural ventilation can underestimate real values twice for low and overestimated twice for very high concentrations. This would have serious safety implications.

Figure 2 (right) shows a functional dependence between the neutral plane height fraction in a vent and hydrogen mole fraction in the enclosure in the assumption of mixture uniformity. For a case of natural ventilation of air, when the hydrogen mole fraction is zero, the half of the vent is occupied by incoming air and another half by outflowing air. The higher the mass flow rate of a leak the higher is the hydrogen mole fraction within the enclosure. The higher the hydrogen mole fraction of hydrogen within the enclosure the lower is the neutral plane location. The curve in Fig. 2 (right) was built using Eq. 10 with calculation of parameter B by Eq. 9 and ρ_{mix} and MF_{H2} by Eqs. 14 and 15 respectively.

3.0 COMPARISON BETWEEN THEORIES AND EXPERIMENT

Figure 3 (left) shows a comparison between maximum measured helium concentrations in experiments [3] and predictions by Eq. 2 for natural ventilation and Eq. 16 for passive ventilation. The discharge coefficient C_D=0.6 is applied in both equations. Experiments [3] were carried out in an enclosure of size $HxWxD$=1.26x0.93x0.93 m with one vent located on a wall near the ceiling. Three different vents were studied: Vent (a) WxH=90x18 cm (A=1620 cm^2), Vent (b) WxH=18x18 cm (A=324 cm^2), and Vent (c) WxH=90x3.5 cm (A=315 cm^2). Release was directed upward from a tube located 21 cm above the floor with internal diameter either D=5 mm or D=21 mm. More details about these experiments can be found in [3].

Figure 3 (left) demonstrates that predictions by the natural ventilation Eq. 2 (dash lines) are far below the experimental data with "normal" C_D=0.6. The predictions of maximum helium concentration by the passive ventilation theory (Eq. 16) are quite close to experimental data throughout the whole range of volume fractions and are on the conservative side. This validates the model as a conservative tool for hydrogen safety engineering to predict maximum concentration in an enclosure (C_D=0.6 to be applied). Figure 3 (right) demonstrates that experimental data on maximum helium concentration in a whole range of conditions [3] are in the limits for the discharge coefficient C_D=0.6-0.95.

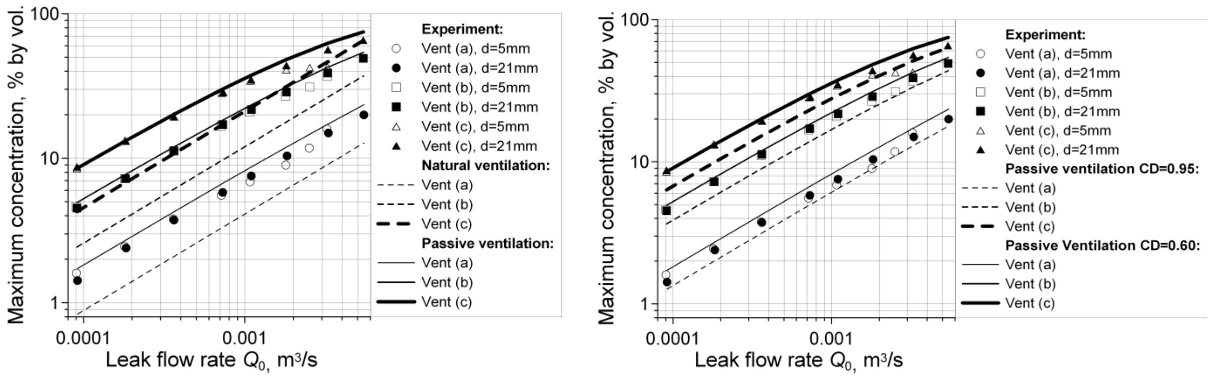


Figure 3. Left: comparison between maximum helium concentrations measured in experiments [3] (points), predictions by Eq. 2 for natural ventilation (dash lines), and by Eq. 16 for passive ventilation (solid lines) with the same discharge coefficient C_D=0.6. Right: comparison between predictions by Eq. 16 for passive ventilation with C_D=0.6 (solid lines) and C_D=0.95 (dashed lines)

To improve the predictive capability of Eq. 2 for natural ventilation an "unrealistic" value of discharge coefficient C_D=0.25 was suggested in study [3]. Figure 4 shows comparison between experimental data and predictions by Eq. 2 with "tuned" C_D=0.25 and predictions by Eq. 16 for passive ventilation with C_D=0.60. While at small concentrations the predictive capability of Eq. 2 with the discharge coefficient C_D=0.25 is improved yet it is hardly acceptable at higher concentrations and especially for horizontal "Vent (c)". In particular, the equation for natural ventilation in the case of "Vent (c)" and leak flow rates above 0.0045 m^3/s "predicts" absolutely unrealistic concentrations above the limit of 100% by volume.

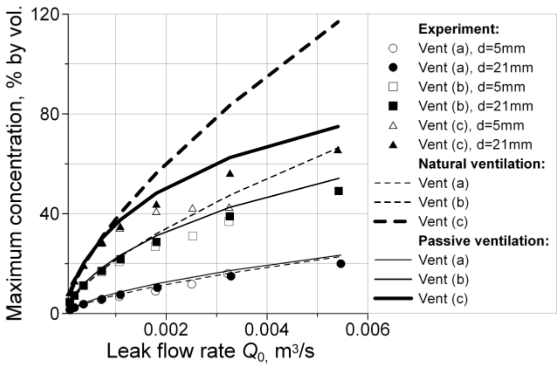


Figure 4. Predictions of experimental data [3] by Eq. 2 for natural ventilation with C_D=0.25 (dash lines), and by Eq. 16 for passive ventilation with C_D=0.6 (solid lines) .

4.0 LEAK FLOW RATE LEADING TO 100% OF GAS ACCUMULATION IN ENCLOSURE

4.1 Equation for Mass Flow Rate Limit leading to 100% Hydrogen Concentration in Enclosure

To exclude air inflow into an enclosure the neutral plane should be at least at the level of lower vent edge or below (Fig. 1, right). When NP is at the lower vent edge, the hydrogen flow rate is at its lower limit that will lead to 100% of hydrogen concentration in the enclosure with time. Indeed, in the beginning of release the jet of hydrogen will entrain air that is initially inside the enclosure and draw it out of the enclosure. Ultimately, with time all air will be removed and pure hydrogen will flow out of the vent to the surrounding atmosphere without air entering the enclosure.

Figure 1 (right) shows a flow of gas out of the enclosure in the limiting case when the neutral plane is at the bottom edge of the vent. The pressure inside and outside the enclosure is $P_{int}(h) = P_{int}^{NP} - \rho_{H2} g(h - h_1)$ and $P_{ext}(h) = P_{ext}^{NP} - \rho_{air} g(h - h_1)$ respectively as $h_{NP} = h_1$. The pressure drop through the vent at height h is $\Delta P(h) = (\rho_{air} - \rho_{H2}) g(h - h_1)$, and the velocity at height h is $U(h) = \sqrt{2\Delta P(h)/\rho_{H2}}$. Integration through the vent height gives the limit of mass flow rate as

$$\dot{m}_{H_2} = W \cdot \int_{h_1}^{h_2} \rho_{H2} U(h) dh = C_D A \sqrt{H} \cdot \sqrt{\frac{8g\rho_{H2}(\rho_{air} - \rho_{H2})}{9}} . \tag{18}$$

The vent area, A, in Eq. 18 after the integration is substituted by $C_D A$ to introduce the discharge coefficient C_D to account for deviations of the assumptions used in the derivation of the model equation from a real 3D flow. The mass flow rate limit is a function of vent height and width only and is not a function of the enclosure volume. The enclosure volume will affect only time required to remove initially present in the enclosure air by entrainment to hydrogen jet and ultimately fill in the enclosure fully by hydrogen. The lower limit for mass flow rate leading to 100% of hydrogen accumulation for a vertical vent is higher than for the horizontal vent of the same area, A. Equation (18) demonstrates that for the same vent area a vent with larger height, H, is more efficient to ventilate gas than a vent with smaller H.

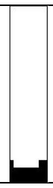
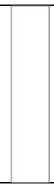
4.2 Verification of the Equation for 100% of Hydrogen Accumulation by CFD Simulations

Numerical simulations were carried out to find out the characteristic value of the discharge coefficient C_D to be applied in Eq. 18 for calculation of the hydrogen mass flow rate limit leading to 100% of hydrogen accumulation in the enclosure. The CFD incompressible solver of the ANSYS FLUENT software based on Reynolds Averaged Navier-Stokes (RANS) equations was applied with the renormalisation group (RNG) k-ε model of turbulence. The calculation domain is a hexahedron of size $LxWxH$=5x2x4 m that included the enclosure of internal size 1x1x1 m (wall thickness of 2 cm) and free space around it. The block-structured hexahedral grid is applied. The total number of control volumes (CVs) is 1,482,475. The total number of CVs in the enclosure is 407,005. The simulations were performed for a vertical vent with cross-section area of HxW=13.9x3 cm and depth of 2 cm. The number of CVs along the vent height is 24, and along the width is 9, the depth of the vent is 4 cells. There are 864 CVs in the vent. Hydrogen was released in simulations upward through a pipe with internal diameter of 5.08 mm located 10 cm above the enclosure floor.

Four simulations were carried out (see Table 1). The mass flow rate was 1.085, 1.204, 1.279 and 1.355 g/s which corresponds to flow velocity at the pipe exit 598.9, 665.4, 707.04 and 748.6 m/s respectively. The simulation were targeting to find the mass flow rate at which the velocity of hydrogen at the bottom edge of the vent is equal or very close to zero for the steady sate conditions. This mass flow rate was then used to calculate the appropriate value of discharge coefficient from Eq. 18. Table 1 includes as well hydrogen concentration in simulations at which calculations were stopped as time of simulations to 100% was impractical.

Simulation results presented in Table 1 show that with hydrogen mass flow rate above 1.279 g/s (velocity 707.4 m/s) there is no air intake into the enclosure. Analysis of simulations confirmed that even at mass flow rate of 1.279 g/s there is small flow velocity through the outer surface of the vent in the direction to the enclosure. However, this little flow entering external surface of the vent is not reaching the internal surface of the vent due to swirling of the flow. In the assumption that flow rate at the lower edge of the vent is equal zero (Eq. 18 is applied) the mass flow rate 1.279 g/s (simulation No.3) corresponds to sought value of C_D=0.85. Thus, we can conclude that for the assessment of the lower limit of mass flow rate that leads to 100% of hydrogen concentration in an enclosure the characteristic discharge coefficient has to be taken as C_D=0.85.

Table 1. Simulation data and velocity distribution through the vent

Simulation	No.1	No.2	No.3	No.4
Mass flow rate, g/s	1.085	1.204	1.279	1.355
Release velocity, m/s	598.9 m/s	665.4 m/s	707.4 m/s	748.6 m/s
Maximum hydrogen concentration, % v/v	97.48	97.54	97.78	98.06
Velocity distribution through the vent perpendicular to the vent outer surface (white colour indicates area with flow out of the enclosure and black colour indicates area with flow into the enclosure).				
Velocity through the outer vent surface, m/s	-0.34÷5.63	-0.26÷5.73	-0.015÷6.08	0.011÷6.49

The vent in simulations was 3D with the depth of 2 cm. Figure 5 shows simulated velocity distribution in a vertical plane of the outer side of the vent as a function of distance, *w*, from the central plane (*w*=0). The velocity distribution confirms that there is no air intake into the enclosure at hydrogen mass flow rate of 1.279 g/s and above, and there is small air intake (small velocities at the bottom edge of the vent) for mass flow rates below this critical value. There is zero velocity on top and bottom edge of the vent surfaces following no-slip boundary condition in simulations. The height where horizontal velocity is zero indicates the location of the neutral plane. In the agreement with analytical model the CFD results show that the neutral plane approaches the bottom edge of the vent with mass flow rate increasing to the limit providing filling the enclosure by leaking gas to 100% by volume concentration.

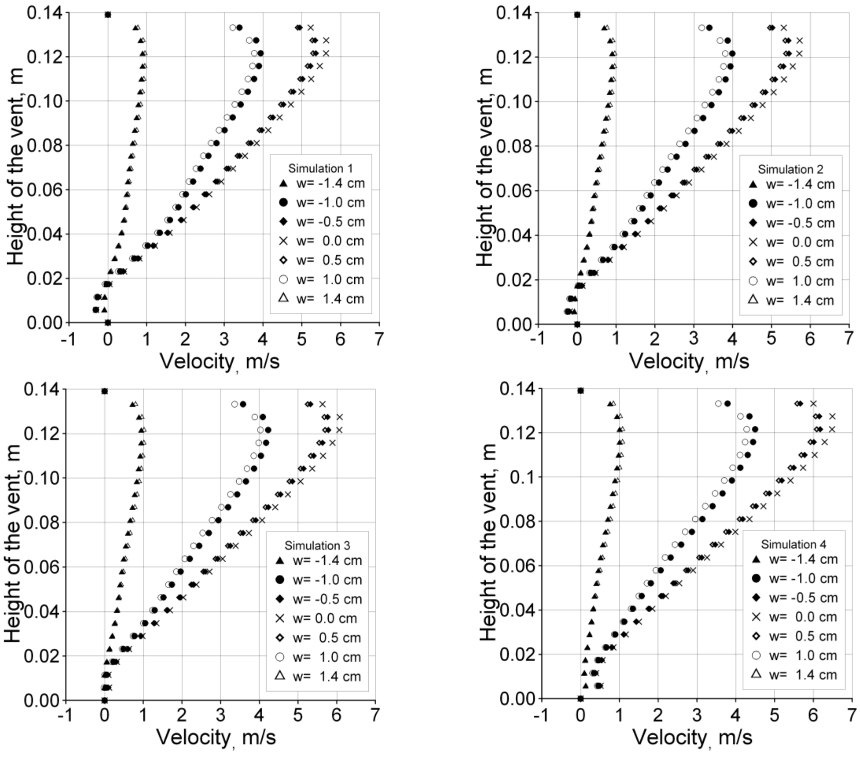


Figure 5. Velocity distribution in a vertical plane of the outer side of the vent as a function of distance, *w*, from the central plane for four simulations (see Table 1)

4.3 Nomogram for Release Flow Rate Limit that Leads to 100% of Hydrogen in Enclosure

Figure 6 shows an engineering nomogram that is a graphical representation of Eq. 18 with determined value of C_D=0.85. The nomogram can be used to calculate a mass flow rate limit by known height and width of a vent, or for calculation of a vent height and width by known hydrogen mass flow rate. For example, a vent with size *HxW*=7x30 cm (see arrows in Fig. 6) will lead to 100% by volume of hydrogen accumulation in an enclosure if a leak mass flow rate is equal or above 3 g/s that is a typical value of hydrogen consumption by a 150 kW fuel cell.

Let us use the nomogram for the inverse problem when the release mass flow rate is known, e.g. 1 g/s. Then, 100% of hydrogen will be accumulated if the vent size is, for example, *HxW*=7x10 cm (not shown in Fig. 6). There are many combinations of vent height and width leading to the same mass flow rate limit. For example, the same leak of 1 g/s would lead to the same result if a narrow vertical vent of size *HxW*=70x0.3 cm is present. However, in the last case the vent area is only 21 cm^2 compared to 70 cm^2 for the former vent size.

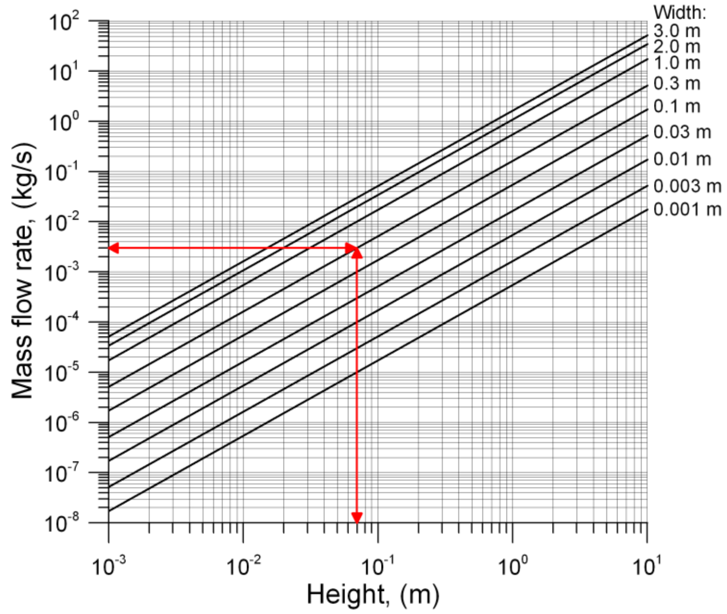


Figure 6. The nomogram for graphical calculation of hydrogen leak mass flow rate in an enclosure with one vent, which leads to 100% of hydrogen concentration, by the vent height and width

5.0 CRITERION FOR MIXTURE UNIFORMITY IN VENTILATED ENCLOSURE

5.1 Previous studies in nominally closed space

In 1994 Cleaver et al. experimentally studied and carried out dimensional analysis of the build-up of concentration within a single enclosed volume following a release of natural gas or propane from nozzles of diameter from 0.6 to 30 mm at pressure from 0.01 to 7 MPa (velocity from 4 m/s to sonic under-expanded jets) [4]. Experiments were conducted in three different enclosures of British Gas of size 3x3x3 m, 3x6x3 m, and 5.4x5.4x2.4 m. They were nominally unventilated with a hole of 12 mm diameter at base to prevent pressurisation. It was established that, in the range of geometrical configurations considered, to a first approximation the gas concentration in the balk atmosphere of the enclosure was uniform across any given horizontal section. Typically, an upper well-mixed layer of constant depth was formed with a lower stratified layer growing beneath it [4]. For any given release from a fixed position in the enclosure, an upward release produces a smaller well-mixed layer than the same release directed horizontally, and the largest well-mixed layer is formed if the release is aimed downwards as observed by Marshall in 1983 [5]. Marshall also noted that whilst changes in the horizontal position of leak within the enclosure produced minor differences in mixing behaviour, the most significant changes arose when the height of the leak above the floor was varied.

Using the analysis by List [6] and Chen and Rodi [7] the length scale after which the momentum-dominated jet becomes buoyancy-controlled plume was given by Cleaver et al. [4] as

$$L = \frac{\alpha \cdot D}{2\sqrt{Ri_N}}, \tag{19}$$

where α is the constant whose value is approximately 1.5, and the Richardson number of the inlet flow

$$Ri_N = \frac{D \cdot g_0^{'}}{2U_N^2}, \tag{20}$$

where U_N is the nozzle velocity, and the reduced gravity is $g_0^{'} = g \mid \rho_a - \rho_g \mid / \rho_g$, in which ρ_g is the density of the gas being released and ρ_a is the density of air initially in the enclosure. Under-expanded jet velocity and radius were calculated in [4] using the pseudo-source (notional nozzle) approach of Birch et al. [8]. For a horizontal release, the jet will turn up at a distance $O(L)$ from the nozzle [4]. For a vertically downwards release, the jet penetrates a distance L before turning upwards. For a vertically upwards jet, at distance L the momentum flux produced by buoyancy is comparable with the initial momentum flux.

Cleaver et al. [4] suggested a parameter which in their opinion provides some measure of the ability of the jet to promote mixing within the nominally closed space with a characteristic size $V^{1/3}$

$$Ri_V = \frac{V^{1/3} \cdot g_0^{'}}{U_N^2}. \tag{21}$$

They argued that this parameter represents the ratio of the potential energy necessary to mix the gas uniformly throughout the enclosure compared with the kinetic energy of the jet. Unfortunately, the Ri_V criterion expressed by Eq. 21 is not applicable to estimate mixture uniformity for ventilated enclosure.

In 1999 Linden [2] described three canonical forms of stratification. Stable stratification when the horizontal interface separates denser fluid below the interface and lighter above the interface. Unstable stratification is characterised by denser fluid being above the interface. The gravity current is another form of stratification when a vertical interface separates regions of different density. Of these three, the stable stratification is the persistent feature, and the other two lead to rapid motion and redistribution of the density field towards the stable case.

5.2 A Criterion for Mixture Uniformity in Vented Enclosure

Let us consider steady-state conditions for a sustained release within an enclosure with one vent. The release provides flow of hydrogen into the enclosure with a constant flow rate. In general case of steady-state distribution of hydrogen within the enclosure with concentration below 100% by volume, there will be a constant flow of air into the enclosure. Thus, the flow of hydrogen and the flow of air into the enclosure will result in a flow of hydrogen-air mixture out of the enclosure. The mixing within the enclosure is mainly due to the entrainment of hydrogen-air mixture into the hydrogen jet that is expected to be momentum-dominated for most of releases from high-pressure equipment.

It is reasonable to assume that the uniformity of mixture within the enclosure will depend on the ratio of the flow rate of mixture entrained into the jet within the enclosure and the flow rate of gases entering the enclosure, i.e. hydrogen from the leak source and air from the outside of enclosure through a part of the vent ($\dot{m}_{mix} = \dot{m}_{H2} + \dot{m}_{air}$). The larger is the venting parameter, $A\sqrt{H}$, the less is the mixture uniformity. The vent area, A, is made dimensional by dividing it by the surface of the enclosure, $V^{2/3}$, and the vent height, H, by the release diameter, D. Based on these assumptions the following uniformity criterion, UC, is suggested that still requires comparison with more measurements, especially in larger volume enclosures, at different conditions of release and ventilation

$$UC = \frac{V^{2/3}\sqrt{D}}{A\sqrt{H}} \frac{\dot{m}_{ent}(x)}{\dot{m}_{mix}}, \tag{22}$$

where the entrainment rate is calculated for a momentum-dominated jet as [9]

$$\dot{m}_{ent}(x) = K_1 M_0^{\ 1/2} \rho_{mix}^{\ \ 1/2} x, \tag{23}$$

and where K_1=0.282 is the constant; ρ_{mix} is the density of the mixture being entrained into the hydrogen jet; x is the distance from the nozzle to the surface of impingement that is typically of the order of distance from floor to ceiling; M_0 is the momentum flux that is equal to

$$M_0 = \frac{\rho_N U_N^2 \pi D^2}{4}, \tag{24}$$

where ρ_{N} is the density of gas at the nozzle.

The uniformity criterion was applied to experimental data [3] on distribution of helium at various conditions of release (volumetric flow rate and release pipe diameter) in the enclosure with one vent of different size (see details in section 3.0). The entrainment rate was calculated by Eq. 23 for all releases (in the assumption that Eq. 23 is applicable). The mass flow rate of hydrogen-air mixture flowing out of the enclosure was calculated by Eq. 3. Experimental data and calculated parameters are given in Table 2 and shown in Fig. 7. The larger the vent the larger is the difference in helium concentration at the top and the bottom of the enclosure. The larger the nozzle diameter the larger is the difference in concentration that is in a full agreement with the similarity law for concentration decay in expanded and under-expanded jets [10]. Figure 7 shows concentrations calculated by Eq. 16 for passive ventilation with two values of the discharge coefficient: C_D=0.60 (conservative estimate) and C_D=0.77 (average value over the range C_D=0.60-0.95, see Fig. 3, right).

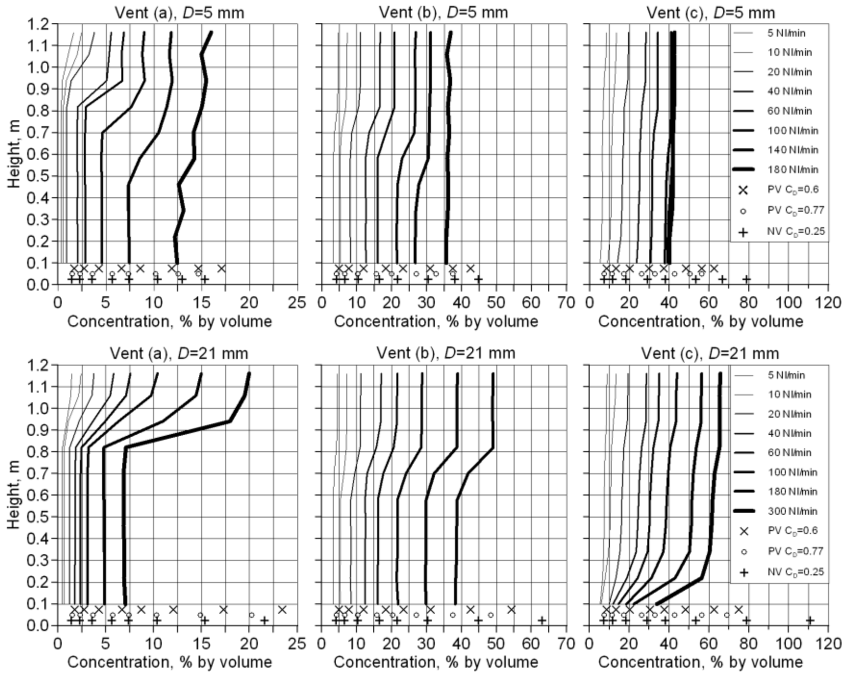


Figure 7. Helium volumetric concentration as a function of height for release through 5 mm pipe (top graphs) and 21 mm pipe (bottom graphs) for Vents (a), (b) and (c) and different flow rates (Nl/min) [3]. Symbols denote helium concentrations calculated by Eq. 2 for natural ventilation with C_D=0.25 ("+") and by Eq. 16 for passive ventilation with the concervative value of C_D=0.60 ("x") and average value of C_D=0.77 ("o")

Table 2. Experimental data [3] and calculated parameters

Vent type HxW D	Experimental data [3]				Calculated parameters					
	Q_0, m^3/s	T_{exp}, K	$C_{\min}$	$C_{\max}$	$X_{\min}/X_{av}$	$X_{\max}/X_{av}$	X	$\dot{m}_{ent}$	$\dot{m}_{mix}$	UC
Vent (a) 18x90 cm 5 mm	9.002E-05	294.9	0.3	1.6	0.534	3.083	0.01354	2.662	7.876	0.357
	1.799E-04	294.7	0.6	2.5	0.608	2.671	0.02140	5.305	9.897	0.567
	3.596E-04	294.5	0.9	3.8	0.620	2.572	0.03375	10.552	12.414	0.899
	7.144E-04	292.6	2.0	5.5	0.674	1.847	0.05283	20.924	15.592	1.419
	1.073E-03	292.8	2.8	6.9	0.707	1.714	0.06871	31.160	17.723	1.859
	1.790E-03	293.1	4.6	9.0	0.742	1.453	0.09535	51.296	20.768	2.611
	2.506E-03	293.2	7.4	11.8	0.781	1.239	0.11793	71.049	23.009	3.264
	3.224E-03	293.4	12.4	16.0	0.887	1.141	0.13801	90.464	24.792	3.856
Vent (a) 18x90 cm 21 mm	9.159E-05	300.0	0.5	1.4	0.676	2.141	0.01369	0.634	7.786	0.176
	1.834E-04	300.4	0.7	2.4	0.646	2.346	0.02167	1.263	9.771	0.280
	3.626E-04	297.0	1.2	3.7	0.686	2.074	0.03393	2.512	12.344	0.441
	7.287E-04	298.4	1.7	5.8	0.635	2.117	0.05351	4.980	15.383	0.701
	1.094E-03	298.8	2.3	7.6	0.649	2.094	0.06961	7.416	17.480	0.919
	1.825E-03	298.9	3.1	10.4	0.645	2.163	0.09654	12.206	20.489	1.291
	3.287E-03	299.1	4.8	15.0	0.654	2.021	0.13966	21.521	24.459	1.906
	5.464E-03	298.3	7.1	20.0	0.666	1.882	0.19049	34.964	28.398	2.666
Vent (b) 18x18 cm 5 mm	8.977E-05	294.1	3.3	4.6	0.873	1.207	0.03902	2.632	2.672	5.207
	1.794E-04	293.9	5.3	7.2	0.879	1.203	0.06123	5.211	3.338	8.253
	3.584E-04	293.6	8.2	11.1	0.884	1.200	0.09544	10.259	4.149	13.067
	7.137E-04	292.3	12.6	16.7	0.884	1.175	0.14695	20.015	5.129	20.621
	1.069E-03	292.0	16.0	20.9	0.882	1.152	0.18804	29.407	5.768	26.934
	1.788E-03	292.9	21.5	26.8	0.888	1.108	0.25461	47.304	6.614	37.774
	2.525E-03	295.5	26.7	31.1	0.912	1.063	0.30951	64.186	7.155	47.364
	3.246E-03	295.4	35.7	36.9	0.988	1.023	0.35481	80.297	7.597	55.788
Vent (b) 18x18 cm 21 mm	9.094E-05	297.9	3.4	4.5	0.896	1.192	0.03935	0.627	2.648	2.563
	1.820E-04	298.1	5.4	7.2	0.872	1.172	0.06179	1.240	3.306	4.065
	3.632E-04	297.5	8.4	11.3	0.879	1.178	0.09624	2.442	4.112	6.432
	7.271E-04	297.8	12.4	17.1	0.871	1.207	0.14864	4.761	5.062	10.187
	1.096E-03	299.4	16.1	21.8	0.875	1.186	0.19089	6.991	5.666	13.361
	1.807E-03	296.0	21.9	28.7	0.885	1.164	0.25615	11.253	6.563	18.559
	3.260E-03	296.7	29.9	39.0	0.889	1.158	0.35567	19.108	7.571	27.302
	5.422E-03	296.1	38.2	49.1	0.887	1.142	0.46118	29.685	8.455	37.950
Vent (c) 3.5x90 cm 5 mm	9.060E-05	296.8	5.2	8.5	0.780	1.272	0.06805	2.597	1.492	21.463
	1.803E-04	295.3	9.1	13.3	0.795	1.168	0.10559	5.105	1.857	33.882
	3.605E-04	295.2	13.8	19.7	0.805	1.149	0.16251	9.930	2.283	53.605
	7.166E-04	293.5	23.6	28.3	0.911	1.093	0.24490	19.023	2.780	84.304
	1.078E-03	294.4	30.5	34.3	0.940	1.059	0.30882	27.520	3.076	110.18
	1.803E-03	295.3	37.6	41.0	0.952	1.037	0.40630	43.160	3.450	153.96
	2.524E-03	295.4	39.4	42.4	0.956	1.030	0.47983	57.400	3.691	191.28
	3.248E-03	295.6	40.3	42.7	0.964	1.023	0.53894	70.521	3.858	224.71
Vent (c) 3.5x90 cm 21 mm	9.088E-05	297.7	6.7	8.7	0.855	1.117	0.06819	0.618	1.489	10.494
	1.825E-04	299.0	7.8	13.2	0.710	1.203	0.10643	1.215	1.841	16.671
	3.639E-04	298.1	13.2	19.4	0.783	1.146	0.16346	2.363	2.268	26.320
	7.341E-04	300.6	18.7	28.6	0.740	1.132	0.24833	4.521	2.731	41.791
	1.091E-03	297.8	24.1	35.0	0.772	1.118	0.31078	6.545	3.049	54.171
	1.806E-03	295.8	31.1	43.9	0.787	1.109	0.40665	10.274	3.446	75.209
	3.266E-03	297.2	43.0	56.3	0.824	1.079	0.54026	16.773	3.840	110.03
	5.406E-03	295.2	56.4	65.8	0.900	1.049	0.66426	25.002	4.164	150.99

Note: T_{exp} is the experimental temperature, C is the helium concentration, % by volume.

The parameters in Table 2 are calculated using the following equations. Densities ρ_{He} and ρ_{air} are calculated by the equation of state $p = (\rho/M)RT$, where pressure was accepted as p=101325 Pa. The helium mass flow rate is equal $\dot{m}_{He} = Q_0 \cdot \rho_{He}$, and the velocity in the nozzle is $U_N = Q_0/A$. Flow rates in Fig. 7 legends are shown in normal litres per minute and the same flow rates are given in Table 2 in cubic meters per second at the experimental temperature. Translation of one to another is done in [3] by multiplying Q_0 in Table 2 by the temperature ratio $273.15/T_{exp}$.

Figure 8 shows experimental values of dimensionless maximum and minimum helium mole fractions [3] as a function of the uniformity criterion defined by Eq. 22. The maximum and minimum mole fractions were dimensionalised by the average concentration calculated using experimental helium distribution in the enclosure. In Fig. 8 curves corresponding to minimum dimensionless mole fractions appear below 1 and maximum – above 1.

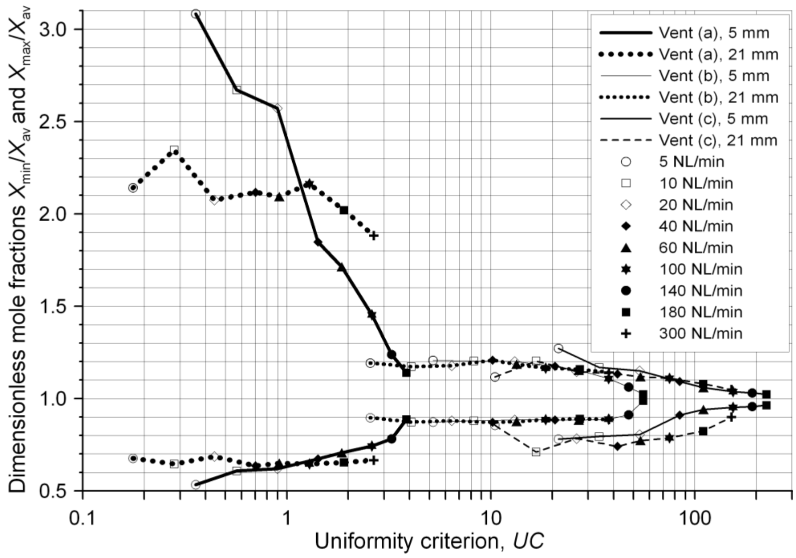


Figure 8. Dimensionless maximum and minimum helium mole fractions in experiments [3] as functions of the uniformity criterion (Eq. 22)

As expected with the increase of the uniformity criterion the difference between maximum and minimum concentrations decreases as a general trend. This is due to better mixing of hydrogen and air entering the enclosure by the entrainment into swirling flow induced by the hydrogen jet or plume. The maximum and minimum mole fractions deviate from its average mole fraction by no more than 20% when the entrainment rate exceeds the mass flow rate of hydrogen-air mixture out of the enclosure to such extent that the uniformity criterion defined by Eq. 22 is UC>4.

6.0 CONCLUSIONS

The model of passive ventilation of sustained gaseous leak in an enclosure with one vent is developed in the assumption of perfect mixing. Equations for passive and natural ventilation are compared. Natural ventilation equations are usually derived in the assumption that the neutral plane is located at or close to the half of the vent height. It is shown that for passive ventilation of accidental release of gas in an enclosure the neutral plane can be located anywhere below the half of the vent height down to the bottom edge of the vent (when the lower limit of mass flow rate leading to 100% concentration of gas in the enclosure will be achieved) and below. It is shown that the exact analytical solution for passive ventilation differs from the approximate solution for natural ventilation by $\pm$2 times. This could have serious safety implications.

The model predictions are compared against experimental helium concentration for both uniform and non-uniform helium-air mixtures in the enclosure of about 1 m^3 volume with one vent of three different sizes and release flow rates in the range from 5 to 300 Nl/min. It has been concluded that the model predictions of concentration are conservative throughout the whole range of tested conditions if the discharge coefficient is C_D=0.60. The best fit values of C_D to reproduce all experiments change from 0.60 to 0.95. The model predictions even with the conservative value of C_D=0.60 are still closer to measured data [3] than estimates by the natural ventilation model with tuned “unrealistic” C_D=0.25.

The equation (18) for calculation of the lower mass flow rate limit of hydrogen that will lead to 100% accumulation of gas in the enclosure is presented and discussed. The equation has only one unknown in advance parameter, i.e. a value of the discharge coefficient. CFD simulations have been performed to find out a mass flow rate that gives zero velocity out of the enclosure at the vent bottom edge. This mass flow rate together with the vent height and width, densities of hydrogen and air were used to derive from the comparison of CFD results and Eq. 18 the value of C_D=0.85. This value is recommended for use in Eq. 18 for 100% hydrogen accumulation. The engineering nomogram to calculate the mass flow rate limit leading to 100% gas concentration in the enclosure as a function of the vent width and height is presented. It follows from the equation that a vertical vent is more efficient for ventilation compared to a horizontal vent of the same area.

The criterion for mixture uniformity in an enclosure with one vent is suggested for the first time. The criterion is the product of three dimensionless ratios: ratio of the entrainment rate to the mass flow rate of the mixture out of the enclosure, ratio of the enclosure surface area to the vent area, and ratio of the release source diameter to the vent height. The maximum and minimum mole fractions deviate from the average mole fraction within about 20% when the criterion value is more than 4.

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