Sustained Hydrogen Leak Concentration in Enclosure with One Vent

Molkov, V.[1]**, Shentsov, V.**[1*] **and Quintiere, J.**[2]

[1] *Hydrogen Safety Engineering and Research Centre (HySAFER), University of Ulster, Shore Road, Newtownabbey, BT37 0QB, UK*
[2] *University of Maryland*
**Corresponding author email: v.molkov@ulster.ac.uk*

ABSTRACT

An analytical model for a steady-state hydrogen concentration during a sustained leak in a passively ventilated enclosure with one rectangular vent is described. An equation for hydrogen concentration in vented enclosure as a function of a leak volumetric flow rate is derived in the assumption of perfect mixing. The predictions by this equation are compared against the experimental data on helium release in 0.97 m^3 volume enclosure and predictions by currently used equation based on the assumptions of natural ventilation of air in buildings. It is underlined that equations derived for natural air ventilation in buildings, which are often built on the equality of volumetric flow rate in and out of the enclosure through a single vent, are not applicable to the design of passive ventilation systems intended to tackle unscheduled hydrogen releases. The difference in concentration predicted by the former natural ventilation equation and the equation for passive ventilation derived here can be as large as ±2 times that has serious safety implications. The developed model predicted the maximum concentrations of helium measured in experiments fairly good in the whole range of test conditions. It can be recommended as a conservative engineering tool for hydrogen safety engineering even for scenarios with non-uniform hydrogen distribution in enclosure with one vent. Besides, an equation for a mass flow rate limit that leads to 100% of hydrogen concentration in a vented enclosure is presented and discussed.

KEYWORDS: Hydrogen concentration, natural and passive ventilation, sustained indoor leak.

NOMENCLATURE

A	vent area (m^2)
B	temporary varaible (-)
C_D	discharge coefficient (-)
g	gravity acceleration (m/s^2)
g'	reduced gravity (m/s^2)
H	vent height (m)
h	height (m)
h_1	distance to a vent bottom edge (m)
h_2	distance to a vent top edge (m)
MF	mass fraction (-)
	mass flow rate (kg/s)
P	pressure (Pa)
Q	flow rate through a vent (m^3/s)
Q_0	release flow rate (m^3/s)
T	temperature (K)
U	velocity (m/s)
V	volume (m^3)
W	vent width (m)
X	volumetric fraction (-)
Greek	
ρ	density (kg/m^3)
Subscripts	
ext	external
H2	hydrogen
int	internal
mix	mixture
NP	neutral plane

INTRODUCTION

Indoor release of hydrogen is a typical scenario of incident with hydrogen and fuel cell systems. There are a number of knowledge gaps in this area of hydrogen safety engineering. One of these

Proc. of the Seventh International Seminar on Fire & Explosion Hazards (ISFEH7), pp. xx-xx
Edited by D. Bradley, G. Makhviladze, V. Molkov, P. Sunderland, and F. Tamanini

ISBN: 978-981-08-7724-8 :: doi: 10.3850/978-981-08-7724-8_0x-0x

gaps is prediction of steady-state concentration of hydrogen sustained leak in an enclosure with one vent. There is a need to develop an analytical model for passive ventilation of enclosure with arbitrary flow rate of a leak. In particular, it is useful to know, when carrying out hydrogen safety engineering, at which sustained (constant) leak flow rate in an enclosure with one vent will be ultimately filled in by 100% of hydrogen.

In 1962 Brown and Solvanson [1] showed that volumetric flow rate Q (m^3/s) through a single rectangular vent of area A (m^2) and height H (m) for natural ventilation in buildings is

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

where C_D is the discharge coefficient; is the reduced gravity in which g is the gravity acceleration, is the density difference, is the average density, and are the densities of the fluid remote from the wall outside and inside the enclosure. The assumption used for derivation of this equation is the equality between volumetric flow rate of air entering and leaving enclosure through a vent. This implies that only half of the vent area is occupied by gases flowing out.

In 1999 Linden [2] dropped 1/3 in Eq. (1) that generated uncertainties in selection of a value of the discharge coefficient C_D by other researchers (three times smaller values of C_D could be expected compared to a typical value C_D=0.6). To carry out comparison with experiments on helium release in one vent enclosure Cariteau et al. re-wrote the equation without 1/3 in terms of the volumetric fraction of hydrogen, X, as [3]

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

where Q_0 is the leak volumetric flow rate, and the reduced gravity is .

MASS FLOW RATE LIMIT LEADING TO 100% OF HYDROGEN IN ENCLOSURE

The neutral plane is a horizontal plane where pressure inside and outside the enclosure are equal, . When the neutral plane is above a lower edge of a vent, the outside air will enter the enclosure below the neutral plane. To exclude air inflow the neutral plane should be at level of the lower vent edge or below. When the neutral plane is at the lower vent edge, the hydrogen flow rate is at lower limit that will lead to 100% of hydrogen concentration in the enclosure with time. Within these assumptions pressures inside and outside the enclosure follow the hydrostatic equation and can be written as , , where h is the height above the lower edge of the vent changing from $h=h_1$ at the lower edge to $h=h_2$ at the upper edge of the vent; h_1 is the height of the lower vent edge above the enclosure floor; are densities outside and inside of the enclosure respectively (Fig. 1, left). Pressure drop through the vent at height h is . Thus, velocity through the vent at a height h can be calculated from Bernoulli's equation as . Integration through the vent height gives

$$\dot{m}_{H_2} = W \cdot \int_{h_1}^{h_2} \rho_{\text{int}} U(h) dh = A\sqrt{H} \cdot \sqrt{\frac{8 g \rho_{\text{int}} (\rho_{ext} - \rho_{\text{int}})}{9}} \,, \tag{3}$$

where W, H and A are width, height, and area of the vent respectively.

Equation (3) shows that the mass flow rate limit is a function of vent sizes only and is not a function of the enclosure volume (densities of hydrogen, , and of air, , are constants). The enclosure volume will affect time required to remove initially present in the enclosure air by entrainment to hydrogen jet/plume and ultimately fill in the enclosure fully by hydrogen. For the same vent area the vertical vent ($H>W$) is more efficient than horizontal vent ($H<W$).

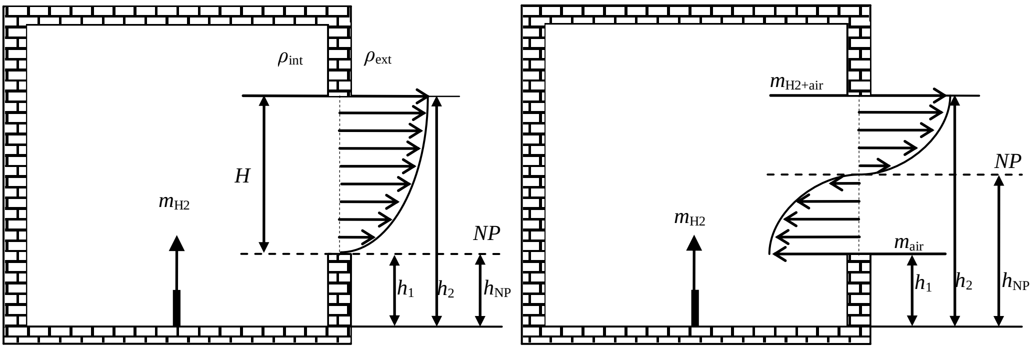

Figure 1. Schematic diagram of the enclosure for a case with the neutral plane at the lower edge of the vent (left); and for a case with the neutral plane between the lower and the upper edge of the vent (right).

STEADY STATE CONCENTRATION OF SUSTAINED HYDROGEN LEAK

Let us now derive a functional dependence between leak mass flow rate, vent sizes (height and width), and steady-state uniform concentration of hydrogen when it is below 100% by volume. In this case the neutral plane will be above of the lower edge and below the upper edge of the vent. The air outside the enclosure will enter the chamber below the neutral plane and lighter hydrogen-air mixture will exit the enclosure above the neutral plane. Figure 1 (right) shows an enclosure schematic diagram of with flows in and out of the enclosure, where h_1 and h_2 are distances from the floor to the bottom edge and to the top edge of the vent, and h_{NP} is the distance from the floor to the neutral plane.

Similar to previous section the pressure inside and outside of the enclosure can be written as , were h changes from $h=h_{NP}$ to $h=h_2$ and where h changes from $h=h_1$ to $h=h_{NP}$ respectively. The pressure difference on the vent is then . The velocities of flowing out mixture and incoming air are and respectively. Integration gives mass flow rates through the vent for hydrogen-air mixture outflow and air inflow

$$\dot{m}_{mix} = W \cdot \int_{h_{NP}}^{h_2} \rho_{mix} dh \cdot U_{mix}(h) = W \cdot (h_2 - h_{NP})^{3/2} \frac{2}{3} \sqrt{2\rho_{mix} g(\rho_{air} - \rho_{mix})}\,, \quad (4)$$

$$\dot{m}_{air} = W \cdot \int_{h_1}^{h_{NP}} \rho_{air} dh \cdot U_{air}(h) = W \cdot (h_{NP} - h_1)^{3/2} \frac{2}{3} \sqrt{2\rho_{air} g(\rho_{air} - \rho_{mix})}\,. \quad (5)$$

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 plus the mass flow rate of the hydrogen entering the enclosure from the leak, i.e. , for the steady-state conditions Therefore, the hydrogen mass flow rate can be obtained by subtraction Eq. (5) from Eq. (4), i.e.

$$\dot{m}_{H_2} = \frac{2}{3} W \sqrt{2g(\rho_{air} - \rho_{mix})} \left[\sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2} - \sqrt{\rho_{air}} (h_{NP} - h_1)^{3/2} \right]. \tag{6}$$

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

$$\dot{m}_{H_2} = W \cdot \int_{h_{NP}}^{h_2} MF_{H_2} \rho_{mix} U(h) dh = \frac{2}{3} W \sqrt{2g(\rho_{air} - \rho_{mix})} \cdot MF_{H_2} \cdot \sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2}. \tag{7}$$

Equating (6) and (7) gives

$$\sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2} - \sqrt{\rho_{air}} (h_{NP} - h_1)^{3/2} = MF_{H_2} \cdot \sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2}, \tag{8}$$

or

$$B = \frac{h_{NP} - h_1}{h_2 - h_{NP}}, \tag{9}$$

where for shortness of calculations B denotes

$$B = \left(1 - MF_{H_2}\right)^{2/3} \left(\frac{\rho_{mix}}{\rho_{air}} \right)^{1/3}. \tag{10}$$

From Eq. (9) the height of the neutral plane is

$$h_{NP} = \frac{h_1 + B h_2}{1 + B}. \tag{11}$$

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 leak. Hence, Eq. (7) can be rewritten as

$$Q_0 \cdot \rho_{H_2} = \frac{2}{3} W \sqrt{2g(\rho_{air} - \rho_{mix})} \cdot MF_{H_2} \cdot \sqrt{\rho_{mix}} (h_2 - h_{NP})^{3/2}. \tag{12}$$

To compare Eq. (2) derived in the assumptions of natural ventilation of air in buildings with Eq. (12) derived for the passive ventilation of hydrogen in enclosure with one vent let us re-write Eq. (12) in the form close to Eq. (2). Firstly, from Eq. (11) bearing in mind that the vent height $H=h_2-h_1$ the following can be derived

$$h_2 - h_{NP} = h_2 - \frac{h_1 + B h_2}{1 + B} = \frac{h_2 + B h_2 - h_1 - B h_2}{1 + B} = \frac{h_2 - h_1}{1 + B} = \frac{H}{1 + B}. \tag{13}$$

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

$$X = \frac{\rho_{air} - \rho_{mix}}{\rho_{air} - \rho_{H_2}}. \tag{14}$$

and thus

$$\frac{\rho_{mix}}{\rho_{air}} = 1 - X \left(1 - \frac{\rho_{H_2}}{\rho_{air}} \right). \tag{15}$$

Mass fraction and volumetric fraction of hydrogen are related through equation

$$MF_{H_2} = \frac{X\rho_{H_2}}{\rho_{mix}}. \tag{16}$$

Finally, Eq. (12) for passive ventilation can be written in the following form convenient for comparison with Eq. (2) for natural ventilation of air in buildings (after the introduction of the discharge coefficient, C_D, as a multiplier to vent area, A)

$$X = f(X)\cdot\left[\frac{Q_0}{C_D A(g^{'}H)^{1/2}}\right]^{2/3}, \tag{17}$$

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

$$f(X) = \left(\frac{9}{8}\right)^{1/3}\cdot\left\{\left[1 - X\left(1 - \frac{\rho_{H_2}}{\rho_{air}}\right)\right]^{1/3} + (1-X)^{2/3}\right\}. \tag{18}$$

PASSIVE VERSUS NATURAL VENTILATION EQUATIONS

Equation (18) describes the function that gives the deviation of exact solution of the problem, i.e. Eq. (17) for passive ventilation, from the approximate solution, i.e. Eq. (2) for natural ventilation of air in buildings. The function is shown in Fig. 2.

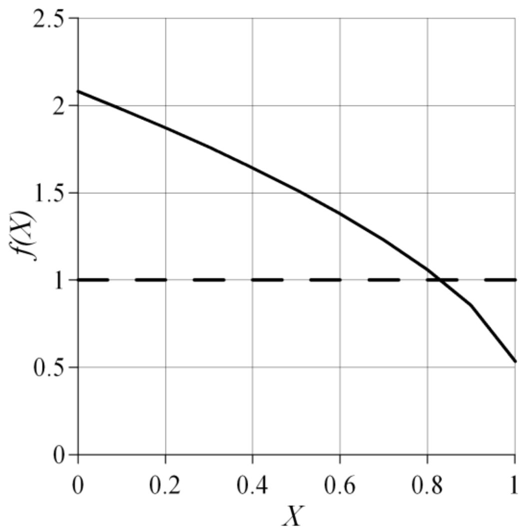

Figure 2. Function $f(X)$ for passive ventilation theory (solid line) and for natural ventilation (dash line).

Figure 2 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 the natural ventilation Eq. (2) can underestimate real values twice for low and overestimated twice for very high concentrations. This would have serious safety implications.

COMPARISON WITH EXPERIMENTAL DATA

Figure 3 shows comparison between maximum measured helium concentrations in experiments [3] and predictions by Eq. (2) and Eq. (17). Experiments were carried out in the enclosure with sizes *HxWxD*=1.26x0.93x0.93 m with one vent located on a wall near the ceiling. Three different vent sizes were studied: vent (a) *WxH*=90x18 cm, vent (b) 18x18 cm, vent (c) 90x3.5 cm. Release was directed upward from a tube located 21 cm above the floor with internal diameter either 5 mm or 21 mm. More details about the experiment can be found in [3].

It is worth noting that predictions are done for the maximum experimental concentrations of helium as both equations are derived in the assumption of mixture homogeneity within enclosure. However, in some tests the distribution of hydrogen was rather layered (non-uniform) than uniform. Nevertheless, the predictions of maximum helium concentration by passive ventilation Eq. (17) are quite close to experimental data throughout the whole range of volumetric fractions. Hence, the model can be recommended for use in hydrogen safety engineering as a conservative tool. More research should be done to, firstly, predict with reasonable accuracy when the mixture can be considered as uniform or layered, and, secondly, to apply after that a theory for uniform (presented here) of layered (to be developed) mixture.

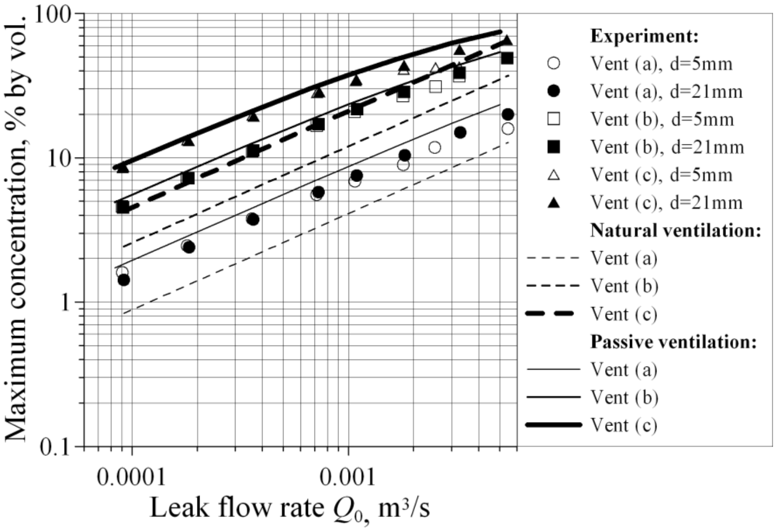

Figure 3. Comparison between experimental data [3] (points), predictions by Eq. (2) for natural ventilation (dash lines), and by Eq. (17) for passive ventilation (solid lines) with the same discharge coefficient C_D=0.6.

Figure 3 demonstrates that Eq. (2) for natural ventilation under predicts measured concentrations significantly if the discharge coefficient C_D=0.6 is applied. To improve the predictive capability of the natural ventilation Eq. (2) "unrealistic" value of discharge coefficient C_D=0.25 was suggested [3].

Figure 4 shows comparison between experimental points and predictions by Eq. (2) with C_D=0.25 and predictions by Eq. (17) with C_D=0.60. While at small concentrations the predictive capability of the "corrected" by the value of discharge coefficient C_D=0.25 Eq. (2) 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 with vent (c) with leak flow rates above 0.0045 m^3/s "predicts" unrealistic concentrations even above the limit of 100%.

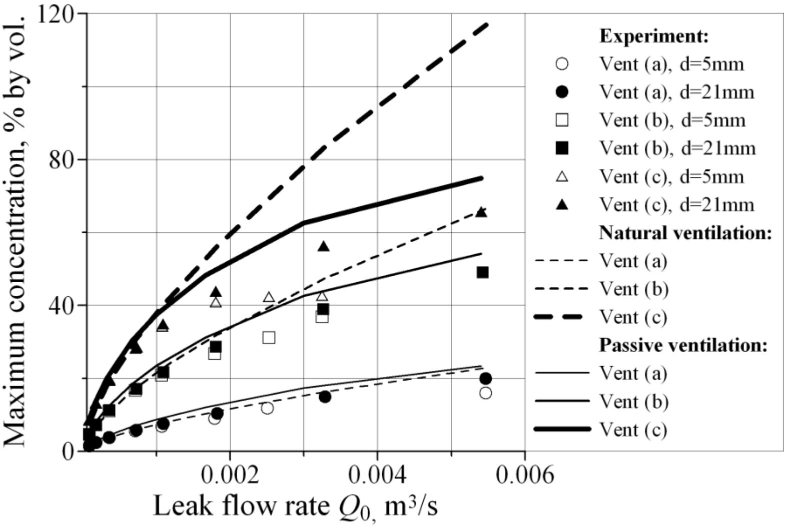

Figure 4. Comparison between experimental data [3] (points), predictions by Eq. (2) for natural ventilation (dash lines) with C_D=0.25, and by Eq. (17) for passive ventilation (solid lines) with C_D=0.6.

CONCLUSIONS

The exact analytical solution for passive ventilation of hydrogen sustained leak in an enclosure with one vent is developed in the assumption of perfect mixing of hydrogen and air within the enclosure. The derived exact solution for hydrogen volumetric fraction during passive ventilation differs from the result predicted by the approximate equation for natural ventilation of air within buildings by $\pm$2 times.

The predictions of maximum helium concentrations measured in experiments [3] by equations for passive and natural ventilation demonstrated that the passive ventilation model predicts experimental data closely in the whole range of tested conditions while the natural ventilation model "overpredicts" the observed concentrations with unrealistic values of concentration above 100% (even with the discharge coefficient C_D=0.25 that was tuned to reproduce closely experiments with small concentrations).

The equation for steady-state concentration of sustained leak predicts well maximum concentrations measured in experiments [3] independent on how uniform were those concentrations. This equation can be applied as a conservative tool to estimate a maximum hydrogen concentration within an enclosure with one vent with a value of discharge coefficient C_D=0.6 for both uniform and stratified (non-uniform) mixtures.

The equation for the mass flow rate limit that leads to 100% of hydrogen in an enclosure with time is derived. This mass flow rate limit is a function of vent area and height only. It does not depend on the enclosure volume. The equation implies that a vertical vent is more efficient for passive ventilation of hydrogen than a horizontal vent of the same area.

ACKNOWLEDGEMENTS

The authors are grateful to Dr Benjamin Cariteau and Dr Gilles Bernard-Michel of CEA (France) for provision and valuable discussions of the experimental data, and to the Fuel Cells and Hydrogen Joint Undertaking for funding of this study under the HyIndoor project (grant agreement number 278534).

REFERENCES

1. Brown, W.G., Solvason, K.R., "Natural convection heat transfer through rectangular openings in partitions. Part I: Vertical partitions", *Int. J. Heat Mass Transfer*, 5 (1962), pp. 859–868.
2. Linden, P.F., "The fluid mechanics of natural ventilation", *Annu. Rev. Fluid Mech*, 31 (1999), pp. 201–238.
3. Cariteau, B., Tkatschenko, I., "Experimental study of the effects of vent geometry on the dispersion of a buoyant gas in a small enclosure", Proceedings of the Fourth International Conference on Hydrogen Safety, September 2011, San Francisco, USA.