

APPLICATION OF NATURAL VENTILATION ENGINEERING MODELS TO HYDROGEN BUILD-UP IN CONFINED ZONES

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ABSTRACT

Correlative engineering models (Linden 1994), are compared to recent published (Cariteau et al. (2009), Pitts et al. (2009), Barley and Gawlick (2009), Swain et al. (1999), Merilo et al. (2010)) and unpublished (CEA experiments in a 1 m³ with two openings) experimental hydrogen or helium distribution in enclosures (with one and two openings). The modelling-experiments comparison is carried out in transient and in steady state conditions. On this basis, recommendations and limits of use of these models are proposed.

1.0 INTRODUCTION

Early (forklifts, backup or base load electricity production...) and mature (cars, buses...) hydrogen energy applications could be localised in confined zones (cabinet, cars, garage...). Natural ventilation is an effective method preventing unacceptable build-up of hydrogen that could induce enclosure destruction and formation of flying fragments in case of ignition and explosion of the flammable. To correctly design the ventilation openings, modelling tools and methods must then be developed. CFD and zonal codes could be helpful for specific and challenging designs but engineering methods will be used for everyday design and risks evaluations.

Hydrogen accumulation modelling in confined zones has been investigated by many researchers. Concerning CFD, some benchmarks have been performed on H₂ build-up in closed enclosure (1, 2). Results are relatively scattered depending on modelling methods and strategies. For the low velocities release, a lot of CFD code fail being predictive.

Zonal models have also been developed (3, 4). These models are based on simple formulation but need a mathematical solving. Published results are generally good.

For air conditioning applications, phenomenological engineering models have been also proposed (5). The models are easy handling and give instantaneous results. The aim of this article is to present the validation of these models against experimental data with hydrogen and helium releases.

2.0 ONE OPENING NATURAL VENTILATION MODEL

2.1 Theory

On the basis of the Linden work, as shown on Figure 1, a well-mixed regime is observed in an enclosure in case of buoyant gas release. Linden (1999) (5) proposes a methodology to calculate the concentration at steady-state and the concentration evolution with time during the filling (during the release) and the drainage phase (after release end).

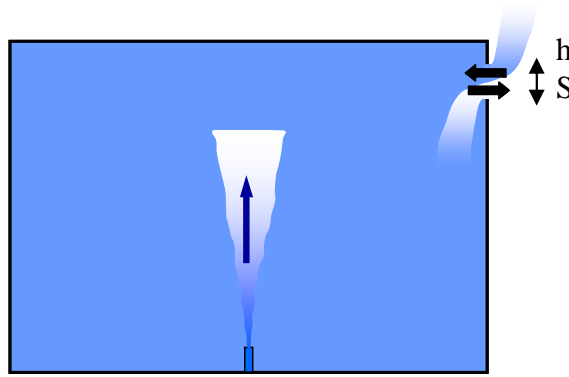


Figure 1. Schematics of the well-mixed regime obtained in case of ventilation by a single opening.

During the filling phase, the expression of the flow crossing the vent opening is given by:

$$Q = C_D S (g'_0 h)^{1/2}, \quad (1)$$

with g'_0 , the reduced gravity ($\text{m}\cdot\text{s}^{-2}$):

$$g'_0 = g \cdot \left(\frac{\rho_a - \rho_0}{\rho_a} \right), \quad (2)$$

where C_D – vent discharge coefficient, constant value, h – vent dimension, m, S – vent area, m^2 , ρ_a – air density, $\text{kg}\cdot\text{m}^{-3}$, ρ_0 – releasing gas (hydrogen) density, $\text{kg}\cdot\text{m}^{-3}$.

It should be noticed that the gas molar fraction is:

$$X_f = \left(\frac{g'}{g'_0} \right), \quad (3)$$

where g' – reduced density of the gas in the enclosure (hydrogen diluted with air), $\text{m}\cdot\text{s}^{-2}$.

Then, if the buoyancy conservation is applied ($g'_0 Q_0 = g' Q$), the fraction of a buoyant gas leading to the steady state in a ventilated room with a single vent is given as follows:

$$X_f = \left(\frac{Q_0}{C_D S (g'_0 h)^{1/2}} \right)^{2/3}, \quad (4)$$

where Q_0 – leaking gas flow rate, $m^3 \cdot s^{-1}$.

The characteristic time scale of filling can be expressed by:

$$\tau = \frac{V}{C_D S (X_f g'_0 h)^{1/2}} \quad (5)$$

The evolution with time of the concentration is given by:

$$\frac{dX^*}{dt^*} = 1 - X^{*3/2}, \quad (6)$$

$$\text{with } X^* = \frac{X}{X_f}, t^* = \frac{t}{\tau}$$

During the drainage phase (i.e. after the end of the gas release), the concentration decreases as follows:

$$\frac{X(t)}{X_i} = \left(1 + \frac{t}{\tau} \right)^{-2}, \quad (7)$$

where X_i – initial concentration at the beginning of the drainage phase, %, τ – characteristic drainage time scale, s.

$$\tau = \frac{2V}{C_D S (X_i g'_0 h)^{1/2}}, \quad (8)$$

where V – volume of the enclosure, m^3 .

2.2 Modelling and experiments comparisons

▪ Cariteau et al. (2011) (6)

In the CEA GARAGE installation (W2.96 x L5.76 x H2.42 m), Cariteau et al. (2011) (6) performed helium dispersion experiments with flow rates from 0.1 to 18 $Nl \cdot min^{-1}$ releasing through a 70 mm nozzle at 0.2 m from the floor. The vent is circular (0.2 m diameter) and localized at 2.22 m from the floor.

The Table 1 gives the comparison between experiments and modelling at steady state. A C_D coefficient of 0.254 was applied to correctly fit the data, which is in very good agreement with the value proposed by Brown and Salvason (1962) (7).

Table 1. Comparison of the experimental data on maximal concentration obtained by Cariteau et al. (2011) and calculated values from the Linden modelling approach (1999).

Q(Nl.min ⁻¹)	%(He) exp.	%(He) calc.
18	8.70	9.89
14	7.69	8.34
10	6.22	6.68
8	5.47	5.76
6	4.76	4.76
5	4.20	4.20
2	2.48	2.29
1	1.96	1.44
0.5	1.24	0.91
0.1	0.68	0.31

A global good agreement is obtained with a bias around 8% and an average absolute deviation of 15% (showing the absence of systematic deviation too).

▪ **Pitts et al. (2009) (8)**

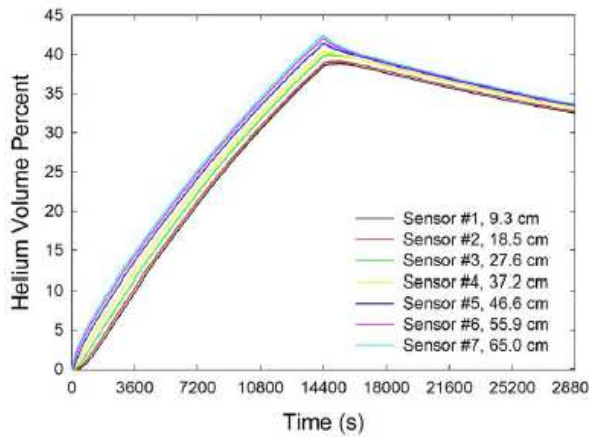
Pitts et al. (2009) (8) carried out helium releases in a ¼ scale two-car rectangular garage (L1.5 x W1.5 x H0.75 m). The box is equipped with one square vent (2.4 x 2.4 cm or 3.15 x 3.15 cm) at 37.5 cm from the floor (in the middle of a face). Helium is released by a Bunsen burner with 3.6 cm diameter opening located 20.7 cm above the floor at the center of the box. Helium flow rates are 14.95 l.min⁻¹ for one hour, and 3.74 l.min⁻¹ for four hours. Helium volume fractions are measured at seven heights using calibrated thermal conductivity sensors.

A comparison of the concentrations at the end of the release is given in the Table 2 for the 4 h experiments.

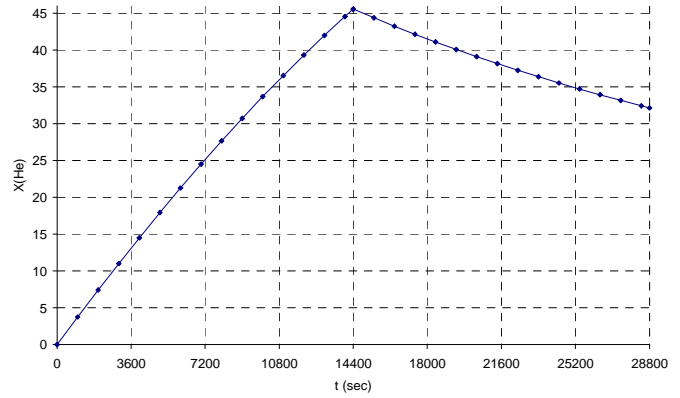
Table 2. Experimental and modelled concentrations for the Pitts et al. experimental conditions (8).

Q ₀ (l/min)	Duration (h)	Vent	%(He) exp.	%(He) calc.
		Height (cm)	at 14 400 s	at 14 400 s
3.74	4	2.4	40-41	45.6
3.74	4	3.15	36-37	40.0

As shown on Figures 2 and 3, a good agreement between calculations and experiments is obtained during the filling and drainage phases. For these calculations, the calculated C_D value (0.254) obtained with the Cariteau experiments is used.

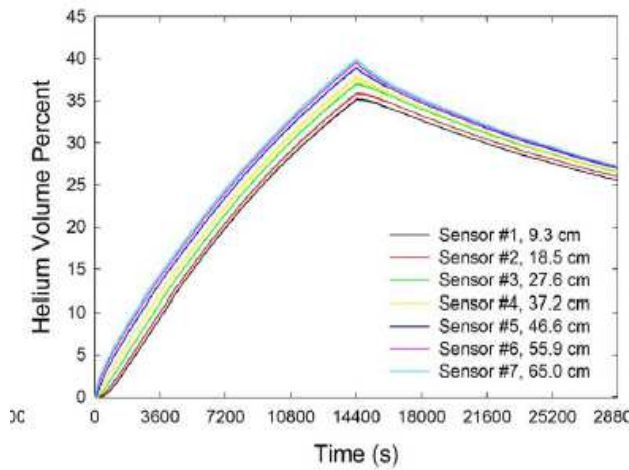


(A)

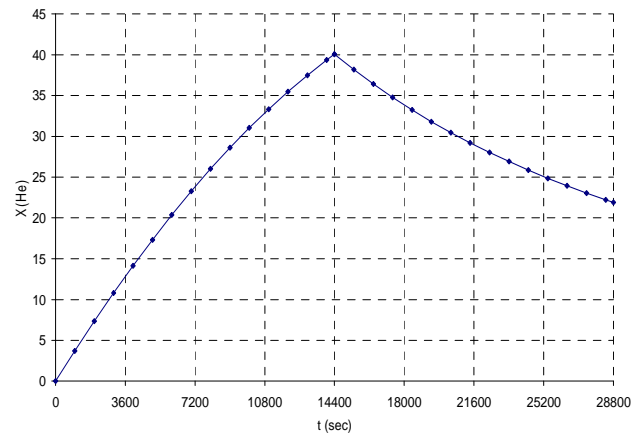


(B)

Figure 2. Comparison of the experimental (A) and calculated (B) concentration evolution during the filling and drainage phases for a 2.4 cm square vent.



(A)



(B)

Figure 3. Comparison of the experimental (A) and calculated (B) concentration evolution during the filling and drainage phases for a 3.15 cm square vent.

2.3 Conclusions

A well mixed regime is obtained in an enclosure ventilated with a single opening without wind. A good agreement is obtained between calculations with Linden method (associated to a discharge coefficient of 0.254) and recently published experiments. This method can be used to size single opening natural ventilation and to calculate concentration reached in an enclosure in case of accidental leak. This model can be used for design, but without any evident limit of use concerning the height of release or the release flow rate.

3.0 TWO-OPENINGS NATURAL VENTILATION MODEL

3.1 Theory

On the basis of the Linden work (5), as shown on Figure 4, a buoyant gas release in an enclosure with two ventilation openings leads to a displacement ventilation regime with the formation of an upper homogeneous concentration. Linden (5) proposes a methodology to calculate the maximal concentration at steady-state.

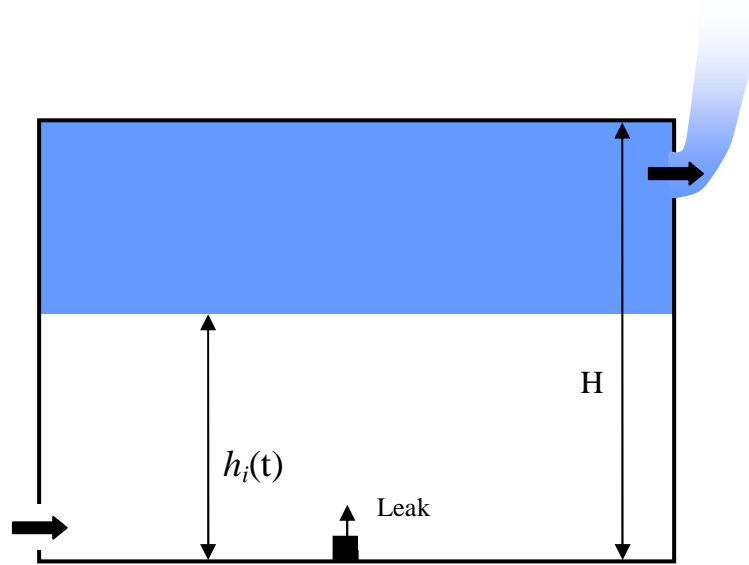


Figure 4. Schematics of the displacement regime obtained in case of natural ventilation by two openings.

Using the S_t and S_b , respectively the opening surfaces of the top and bottom openings, the effective opening area is:

$$S' = \frac{\sqrt{C_t S_t S_b}}{\left(\frac{1}{2} \left(\frac{C_t}{C_b} S_t^2 + S_b^2 \right) \right)^{1/2}}, \quad (9)$$

where C_t – top vent discharge coefficient, constant value, C_b – bottom vent discharge coefficient, constant value, constant value, S_t – top vent area, m^2 , S_b – bottom vent area, m^2 .

At steady state, the interface height, h_i , is given by:

$$\frac{S'}{H^2} = C^{3/2} \left(\frac{\xi^5}{1-\xi} \right)^{1/2}, \quad (10)$$

and:

$$\xi = \frac{h_i}{H}, \quad (11)$$

where H – height of the enclosure, m.

The height of the interface only depends on the geometrical configuration of the vents (size and height).

At steady state, the molar fraction in the upper layer is expressed by:

$$X_f = \frac{1}{C} \left(\frac{Q_0^2 h_i^{-5}}{g_0'} \right)^{\frac{1}{3}}, \quad (12)$$

where g_0' – reduced gravity, m.s^{-2} , C – constant value of 0.115 depending on the air entrainment coefficient α (0.10 is used herein for α in Linden approach formulation):

$$C = \frac{6}{5} \alpha \left(\frac{9}{10} \alpha \right)^{\frac{1}{3}} \cdot \pi^{\frac{2}{3}} \quad (13)$$

It is important to notice that in this model the release is considered on the floor.

3.2 Modelling and experiments comparisons

▪ CEA GARAGE experiments

Experiments were performed with helium release in the GARAGE facility (L5.76 x W2.96 x H2.42 m). The garage is equipped with two circular vents (0.2 m diameter) located at 0.22 and 2.22 m from the floor. Helium is released by a 70 mm diameter orifice at 0.20 m from the floor. With the vent location and size, a homogeneous layer is calculated at 0.93 m above the floor.

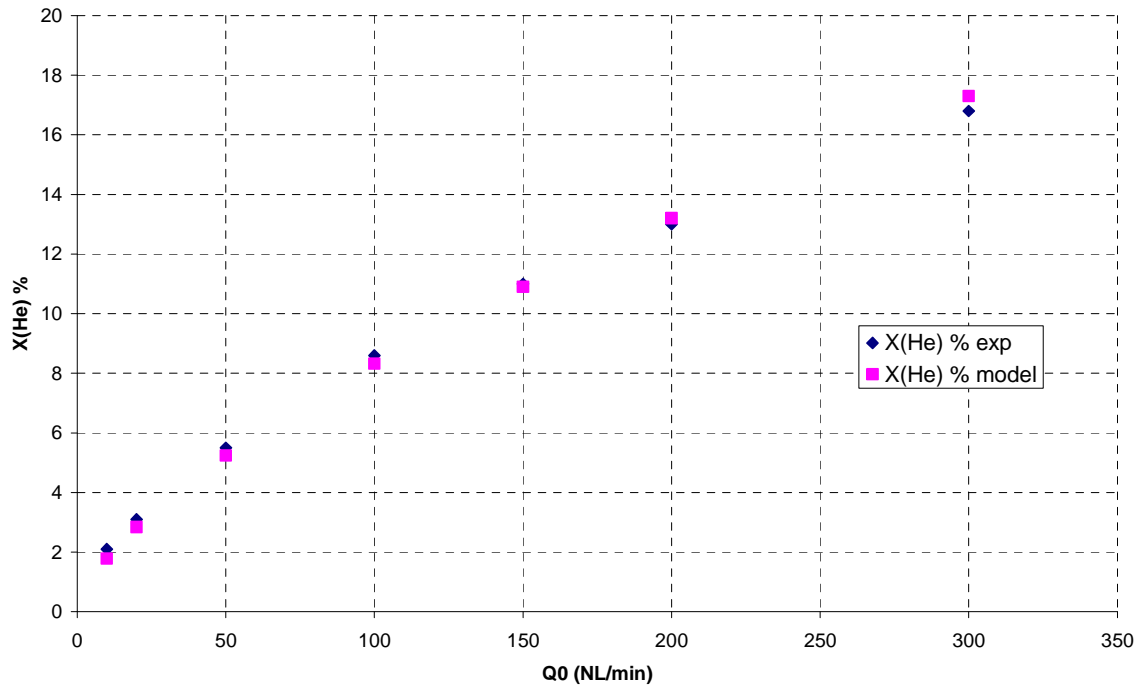


Figure 5. Calculated and experimental steady state concentrations.

As shown on Figure 5, a very good agreement is obtained between experiments and modelling with an average deviation less than 9%.

To obtain this agreement, a value of 0.5 is used for C_t and C_b . These values are kept constant in the following paragraphs. These values of discharge coefficient for two openings configuration are larger than the previous value for one opening configuration because in the well-mixed regime – previously treated – the ventilation vent is both used to introduce fresh air and to remove hydrogen-enriched air.

▪ **Pitts et al. (2009) (8)**

Pitts et al. (8) also carried out helium releases in a box (L1.5 x W1.5 x H0.75 m) equipped with two square vents (2.15 x 2.15 cm) at 2.5 cm and 72.5 cm from the floor. Flow rates (diameter 3.6 cm at 20.7 cm above the floor at the center of the box) are $14.95 \text{ l}\cdot\text{min}^{-1}$ for one hour and $3.74 \text{ l}\cdot\text{min}^{-1}$ for four hours. According to the authors, laboratory and gas temperatures were maintained at 21°C .

A comparison of the concentrations at the end of the release is given in the Table 3.

Table 3. Experimental and modelled concentrations for the Pitts et al. experiments (8).

Q_0 (Nl.min ⁻¹)	Duration (h)	%(He) exp.	%(He) calc.
3.47	4	17	19.1
13.84	1	35	48.1

As shown on Figure 6, the concentration after a 4 h (14 400 s) release is at steady state and is then really comparable to the calculations. A relatively good experiment-calculation agreement is obtained. The calculation for the one hour release is only given for information because steady state was not reached.

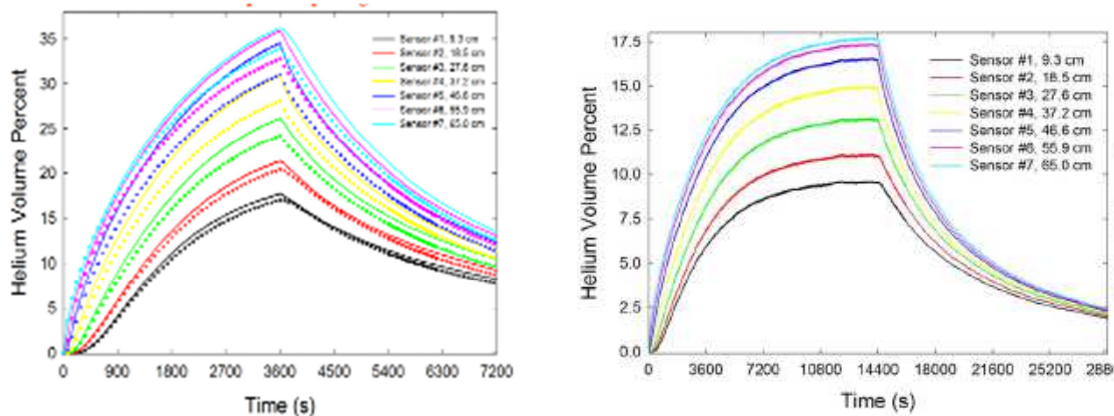


Figure 6. Comparison of the transient concentrations profiles for the Pitts et al. experiments (8).

▪ **Barley and Gawlick (2009) (9)**

Barley and Gawlick (9) performed helium releases experiments in a rectangular room (L7.02 x W4.29 x H2.74 m). This room is placed in a big hall avoiding wind effects. The lower and

upper ventilation openings (W32.4 x H24.3 cm) are located at 0.37 and 2.38 m from floor, on the same wall.

The leak was located at variable height above the center of the test room floor (Y_s in Table 4). The injection system is a local diffuser (automobile oil filter element, 9.6-cm height and 8-cm diameter) or a line diffuser (1.83-m length porous hose). These configurations are respectively noted P and L in the Table 4.

The Table 4 gives the steady state concentrations in the homogenous upper layer.

Table 4. Experimental (9) and modelled steady state concentration values.

Case	Y_s (m)	Q_0 (NI.min-1)	%(He) exp.	%(He) calc.
P1	0.61	9.0	1.2	0.9
P2	0.61	20.2	2.0	1.5
P3	0.61	37.1	2.9	2.3
P4	0.91	11.3	1.5	1.0
P5	0.91	22.6	2.6	1.6
P6	0.91	17.0	2.7	1.3
L1	1.22	20.3	1.7	1.5
L2	0.61	37.3	2.4	2.3

A rather good agreement is obtained between experiments and modelling even if the calculated results are always below experiments. The average absolute deviation is about 26%. It is noteworthy that increasing the height of the source leads to an increase in the concentration. The model could be easily enhanced by taking into account the source height.

▪ **Swain et al. (1999) (10)**

Swain et al. performed helium and hydrogen release experiments in a rectangular corridor (L2.99 x W0.74 x H1.22 m) (10). The setup is equipped by two rectangular vents (L30.48 x H15.24 cm) on the roof and on the door. The release flow is 52.76 NI.min⁻¹ during 20 min by a rectangular vent (L30.48 x H15.24 cm) located on the floor.

Using the Linden model, the calculated steady state concentrations in the upper layer are 5.94 and 6.09% respectively for hydrogen and helium experiments, which is in good agreement with the 5% concentration reported by Swain.

▪ **Merilo et al. (2010) (11)**

Merilo et al. (11) carried out hydrogen releases in an experimental garage (H2.72 x W3.63 x L6.10 m). The lower vent is a rectangular vent (L1.22 x H0.09 m) near the floor and the upper vent is circular (0.11 m²) at 2.42 m from the floor. Two hydrogen flow rates were tested: 9.22 kg.h⁻¹ and 0.88 kg.h⁻¹ (respectively 1722 and 164 NI.min⁻¹) by a 7.75 mm inner-tube diameter at 1 m from the floor.

As shown in Table 5, a reasonable agreement is obtained between experiments and Linden calculated upper layer concentrations even if wind effects are not taken into account in the model.

Table 5. Experimental and modelled steady state concentrations (11).

Q_0 (Nl.min ⁻¹)	%(H ₂) exp.	%(H ₂) calc.
1722	23	23.5
164	7.1	4.9

3.3 Conclusions

A displacement regime characterised by the formation of a homogeneous upper layer is obtained in an enclosure naturally ventilated with two openings without wind. A good agreement is observed between calculations obtained by Linden approach and recently published experiments.

4.0 OVERALL CONCLUSIONS

The engineering models proposed by Linden to calculate the evolution of the concentration of hydrogen in an enclosure naturally ventilated with a single or two openings without wind effects have been evaluated.

With only one ventilation opening, a well-mixed configuration with a homogenous gas concentration in the enclosure is described. In this configuration, a good agreement is obtained between calculations performed with Linden method and recently published experiments.

With two openings, displacement regime with formation of a homogenous upper layer is observed. A good agreement is also obtained between Linden based calculation method and recent experiments.

These two methods can be used to size natural ventilation openings and to calculate concentration reached in an enclosure in case of accidental leak, provided that the main hypothesis of the models are valid That is to say, the leak should be close to a plume and at a level close to the floor in the case of the displacement regime (two vents configuration).

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REFERENCES

1. Venetsanos, A.G., Papanikolaou, E., Delichatsios, M., Garcia, J., Hansen, O.R., Heitsch, M., Huser, A., Jahn, W., Jordan, T., Lacombe, J.M., Ledin, H.S., Makarov, D., Middha, P., Studer, E., Tchouvelev, A.V., Teodorczyk, A., Verbecke, F. and Van der Voort, M.M., An inter-comparison exercise on the capabilities of CFD models to predict the short and long term distribution and mixing of hydrogen in a garage, *International Journal of Hydrogen Energy*, **34**, N°14, 2009, pp. 5912-5923.
2. Bernard-Michel, G., Cariteau, B., Trochon, J., Jallais, S. and Vyazmina, E., CFD benchmark based on experiments of helium dispersion in a 1 m³ enclosure - intercomparisons for plumes and buoyant jets, ICHS5, September 2013, Brussels.

3. Lowesmith, B.J., Hankinson, G., Spataru, C. and Stobbart, M., Gas build-up in a domestic property following releases of methane/hydrogen mixtures, *International Journal of Hydrogen Energy*, **34**, N°14, 2009, pp. 5932-5939.
4. Prasad, K., Pitts, W.M. and Yang, J.C., A numerical study of the release and dispersion of a buoyant gas in partially confined spaces, *International Journal of Hydrogen Energy*, **36**, N°8, 2011, pp. 5200-5210.
5. Linden, P., The Fluid Mechanics of Natural Ventilation, *Annu. Rev. Fluid Mech.*, **31**, 1999, pp. 201-238.
6. Cariteau, B., Brinster, J. and Tkatschenko, I., Experiments on the distribution of concentration due to buoyant gas low flow rate release in an enclosure, *International Journal of Hydrogen Energy*, **36**, N°3, 2011, pp. 2505-2512.
7. Brown, W.G. and Solvason, K.R., Natural convection through rectangular openings in partitions, *Int. J. Heat Mass Transfer*, **5**, 1962, pp 859-868.
8. Pitts, W., Yang, J. and Prasad, K., Experimental Characterization of a Helium Dispersion in a ¼ Scale Two-Car Residential Garage, *IEA Hydrogen Implementing Agreement Task 19 Experts Meeting*, 2009.
9. Barley, C.D., and Gawlik, K., Buoyancy-Driven Ventilation of Hydrogen from Buildings: Laboratory Test and Model Validation, *International Journal of Hydrogen Energy*, **34**, No 13, 2009, pp. 5592-5603.
10. Swain, M.R., Filoso, P., Grilliot, E.S. and Swain, M.N., Hydrogen Leakage into Simple Geometric Enclosures, *International Journal of Hydrogen Energy*, **28**, No. 2, 2003, pp. 229-248.
11. Merilo, E.G., Groethe, M.A., Colton, J.D. and Chiba, S., Experimental Study of Hydrogen Release Accidents in a Vehicle Garage, *International Journal of Hydrogen Energy*, **36**, No. 3, 2011, pp. 2436-2444.