

PERFORMANCE COMPARISON OF HYDROGEN DISPERSION MODELS IN ENCLOSURE ADAPTED TO FORCED VENTILATION

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ABSTRACT

In confined spaces, hydrogen released with low momentum tends to accumulate in a layer below the ceiling; the concentration in this layer rises and can rapidly enter the flammability range. In this context, ventilation is a key safety equipment to prevent the formation of such flammable volumes. To ensure its well-sizing to each specific industrial context, it is necessary to dispose of reliable engineering models. Currently, the existing engineering models dealing with the buoyancy-driven H₂ dispersion in a ventilated enclosure mainly focus on the natural-ventilation phenomenon. However, forced ventilation is in some situations more adapted to the industrial context, as the wind direction and intensity remains constant and under control. Therefore, two existing wind-assisted ventilation models, elaborated by Hunt and Linden [1] and Lowesmith et al. [2], were tested on forced ventilation applications. The main assumption consists in assuming a blowing ventilation system rather than a suction system, as the composition and velocity of the entering air are known. The fresh air enters the down opening and air-hydrogen mixture escapes through the upper one. The adapted models are then validated with experimental data, releasing helium rather than hydrogen. Experiments are conducted on a 1-m³ ventilated box, controlling the release and ventilation rates. The agreement between both analytical and experimental results is discussed from the different comparisons performed.

1.0 INTRODUCTION

In the current energy transition context, hydrogen is expected to play a key role. The number of its potential applications and usages is increasing (for example the mobility, the energy storage or the industry), while the demand as well as the production capacities are exploding.

The generalisation of the use of hydrogen and the expansion of its market enhances the concern of the safety. Indeed, hydrogen is a highly flammable product, due to both its flammability range (4 to 77 % in the ambient air) and to the low level of energy required to start its ignition (20 μJ, being 10 times lower than hydrocarbons like methane). Therefore, it is essential to anticipate the pain points in terms of safety and find beforehand prevention and mitigation solutions.

Among the most critical configurations in terms of safety, we can find the case of an accidental release in confined spaces. Being unable to disperse in the atmosphere, the hydrogen is going to accumulate in the building and mix with the ambient air. Hence, its concentration is likely to rise rapidly and to overpass short after the release start the level of the lower flammability limit. This phenomenon is enhanced by its low molecular weight and its high buoyancy, leading to its accumulation in a layer high up under the ceiling, as described in numerous papers [3] [4] [5]. Such a situation can typically be found in the industry (release from leaking plugs or vessels inside a plant) or in the mobility (hydrogen leakage from the vehicle's reservoir parked in a garage).

The most efficient way to prevent the formation of such a hazardous H₂ layer is the ventilation of the enclosure so that the released hydrogen can be removed outside and replaced by fresh air. The ventilation can be either naturally or mechanically driven. In the first case, the walls of the enclosure dispose of one or several openings through which the hydrogen and the fresh air respectively flow outward and inward

due to a natural pressure difference. The second case (also called forced ventilation) generally corresponds to an extraction system of the upper layer while fresh air naturally enters the enclosure through a bottom opening. To ensure the safety of the installations, it is important to size adequately the ventilation system and hence to dispose of reliable models of dispersion in a ventilated enclosure. The existing models can be either numerical (CFD models) [6] [7] or analytical (engineering models) [1] [2] [3].

More simple and faster, analytical models are best suited to releases occurring in standard building geometries. They were commonly developed for low-momentum releases in unventilated or naturally ventilated enclosures. This article aims to compare the relevance of such models, as they are applied on a mechanically-driven ventilation case. In this purpose, the adaptation of both analysed models developed by Hunt and Linden [1] and Lowesmith et al. [2] to mechanical ventilation is presented in section 2.0. Then the experimental platform for dispersion in a confined mechanically ventilated enclosure is presented in section 3.0 and the validation of the analytical models against the test results is performed in section 4.0.

2.0 CONSIDERED ANALYTICAL DISPERSION MODELS

The dispersion of a light gas in an enclosure can lead to multiple hydrogen distributions: a well-mixed distribution [8], a 2-layered distribution with a constant concentration in the upper layer, a 2-layered distribution with a non-homogeneous upper layer [4], a 3-layered distribution [3]... In this paper, we focus on the stratification phenomenon with constant distribution in the upper layer, as described in the models of Hunt and Linden [1] and Lowesmith et al. [2].

Both of them are based on a buoyancy-driven dispersion assisted by the wind in a two-opening parallelepipedic enclosure: they assume a bottom opening on the windward side of the enclosure and a top opening placed on the leeward façade. The light gas is released at a given height in the center of the box, so that the release flow is not disturbed by the enclosure vertical walls and escapes through the upper opening. In the models adaptation, such a configuration is kept, the ventilation system is represented by a flow rate, which can be, knowing the size of the openings, translated into a velocity. However, to simplify the modelling, we considered for both models a blowing rather than an extracting ventilation system. Such an assumption is important as the inlet velocity remains constant (ambient conditions are not supposed to change) whereas the outlet velocity is influenced by the density of the mixture in the upper layer and thus by its hydrogen concentration.

2.1 Linden modelling [1]

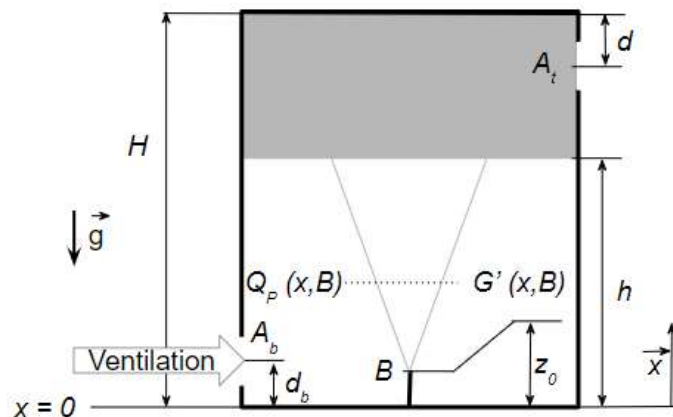


Figure 1. Schematic representation of the modelling according to the Linden model

Linden et al. [9] initially developed a mathematical modelling about the behaviour of light gas released in a naturally ventilated enclosure disposing of one or two vents without considering the wind effects. The dispersion phenomena are not handled similarly depending on the number of openings: in case of a

single opening (placed on top), the light gas mixes in the whole volume of the box (mixing ventilation), whereas with two openings, a stratification appears with an upper layer rich in light gas and a bottom layer free of it (displacement ventilation). The wind effects have been added only in the case of displacement ventilation, whether assisting the buoyancy [1] or opposing to it [10].

The displacement ventilation modelling assumes a top-hat profile for the density and the velocity across the buoyancy-driven plume (buoyancy B assumed constant) and adopts the Boussinesq approximation. It also supposes that the mixture outflow at the top opening is governed by the difference of hydrostatic pressure, whereas the air inflow (wind) depends on the dynamic pressure drop between the windward and leeward openings; the wind coming from the bottom opening assists here the stratification. Therefore, Linden's model proposes a single non-linear equation to solve on the layer interface height at steady state:

$$\frac{A^*}{H^2} = \frac{C^{3/2} \zeta^{5/3}}{\sqrt{\frac{1-\zeta-(d+z_0)/H}{\zeta^{5/3}} - C Fr^2}} \quad (1)$$

Where:

- $\zeta=h/H$ corresponds to the unknown relative height of the interface (h being the actual height of the interface at steady state).
- $Fr = \sqrt{\frac{\Delta}{\rho}} / \left(\frac{B}{H}\right)^{2/3}$ corresponds to the Froude number, namely a ratio of the buoyancy forces compared to the ventilation forces: if $Fr \ll 1$, buoyancy forces are dominant whereas ventilation forces dominate for $Fr \gg 1$. Here, Δ refers to the wind pressure drop, related to the wind velocity, and ρ to the mass density of the ambient air.
- A^* is designated as an 'effective opening': it represents the energy losses of the flowing fluid through the top and bottom openings. It is calculated by taking into account the inlet and outlet areas of the openings (A_b and A_t respectively) and the coefficients of expansion and discharge through these openings (C_e and C_D respectively): $A^* = A_b A_t \sqrt{\frac{2 C_e C_D^2}{C_e A_b^2 + C_D^2 A_t^2}}$.
- $C \approx 0.14$ is a parameter dependent upon the top-hat entrainment coefficient of the plume.

From this equation, the light gas concentration in the upper layer can be deduced:

$$X_{Lind} = \frac{1}{C} \sqrt[3]{\frac{Q_{rel}^2}{g'_0 (h-z_0)^5}} \quad (2)$$

With $g'_0 = g (\rho - \rho_{lg})/\rho$ reduced gravity of the released light gas (mass density ρ_{lg}).

Such a modelling can be easily adapted for a blowing ventilation system, converting the wind velocity into an inlet flow rate Q_{vent} .

2.2 Lowesmith modelling [2]

This modelling approach was developed for the wind-assisted light-gas dispersion in the so-called displacement ventilation configuration. On the contrary to the Linden model, this one is not restricted to the final state but deals with the transitional period. It assumes initially that the enclosure is filled with ambient air and is continuously ventilated, before the release of the light gas starts; the released gas immediately accumulates in a layer below the ceiling due to its buoyancy enhanced by the wind effect. The layer gets thicker up to a final state where the amount of light gas entering it due to the release is balanced by the amount of outflowing gas through the opening in contact.

The modelling is performed into two successive steps:

- The first one determines the flow rate of the air-light gas mixture entering the upper layer Q_j depending on the difference of height between the layer interface and the release point. The model of a buoyant jet developed by Lane-Serff and al [11] is applied, based on the Boussinesq approximation and supposing that the entrainment into the jet is proportional to the local mean jet velocity. A system of spatial differential equations has to be solved:

$$\begin{cases} \frac{d}{dz}(U_j R^2) = 2 R \alpha U_j \\ \frac{d}{dz}(U_j^2 R^2) = g'(\lambda R)^2 \\ \frac{d}{dz}(g' U_j R^2) = 0 \end{cases} \quad (3)$$

Where the unknown respectively U_j , R and g' designate the local mean jet velocity, the local jet radius and the local reduced gravity at the height z from the release source, while α and λ are constants.

- The second step aims to calculate at each time step the thickness of the light gas enriched layer $S(H_1 + d)$ and its concentration X . The system of equations to solve is a mass and volume balance:

$$\begin{cases} S \frac{d}{dt}(H - h - d) = Q_j - Q_{in} - Q_{rel} \\ S (H - h - d) \frac{d}{dt}(X) = Q_{rel} - X Q_j \end{cases} \quad (4)$$

Where $Q_j(z) = \pi R^2(z) U_j(z)$ is the volume flow rate of the air-light gas mixture entering the layer located at a height z above the release point ($z = h - h_0$), Q_{in} is the volume flow rate of the air entering the enclosure, function of the natural ventilation and the wind flow rates, and Q_{rel} represents the release flow rate of the light gas ($Q_{rel} = Q_S$ in Figure 2).

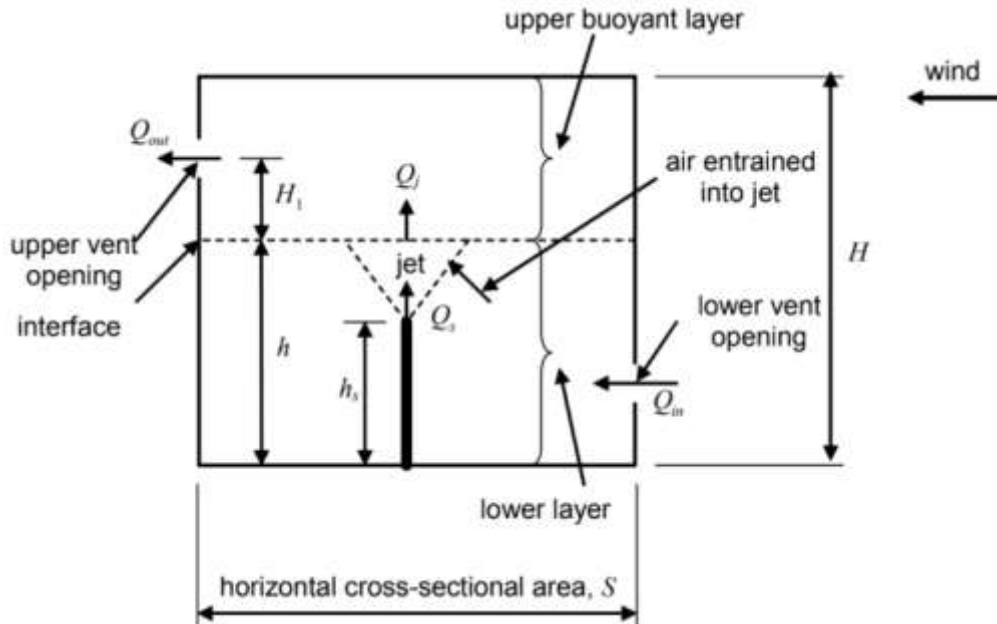


Figure 2. Schematic representation of the modelling according to the Lowesmith et al. [2]

This second model does not require any special modification to be adapted to mechanical ventilation.

3.0 EXPERIMENTAL PLATFORM FOR DISPERSION TESTS

To validate the models, experimental tests have been performed on a platform of light-gas dispersion elaborated at the Innovation Campus Paris. As presented in Figure 3, it consists in a 1 m³ cubic box (horizontal area 1 m²), at the center of which the light gas is released through a circular nozzle oriented upwards. The release rate is mastered with a flowmeter (Brooks SL5853) yearly calibrated and takes place at a previously defined height. The release flow rate of the light gas can go up to 600 NL/min.

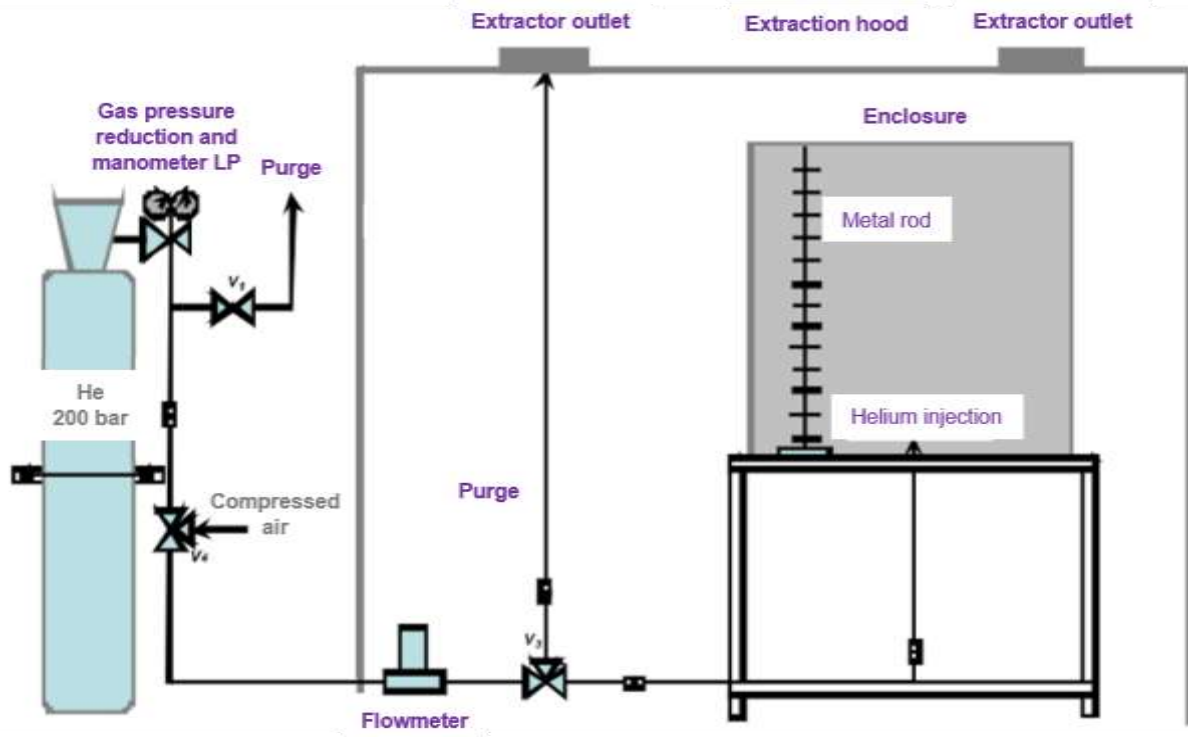


Figure 3. Schematic representation of the platform used for the light gas dispersion tests [14]

To dispose of accurate data on the dispersion of hydrogen in an enclosure, it would have been worthwhile to use it as the released light gas. However, due to its inherent hazards, hydrogen is replaced by helium for safety reasons. The literature has confirmed that such a solution is relevant, providing comparable results for both fluids [12] and has been applied in other experiment campaigns following a similar protocol [5] [8] [13].

The concentration of the light gas is recorded live every second at several heights with the help of catharometers (Xensor Xen-TCG 3880) specifically calibrated for helium concentration measurements and vertically disposed every 6.5 cm on a metal rod. Catharometers are working as a Wheatstone bridge. They measure the thermal conductivity difference between the gaseous environment and a gas reference, which induces a temperature gradient and thus a resistance difference in the electric apparatus; this resistance difference is correlated with a concentration of the helium in the air (absolute accuracy 0.02 % within the range 0 – 40 % of He in the air). Doing so, the evolution of the helium concentration at a given height as well as the vertical distribution of the dispersed helium at steady state can be observed for comparison with the models.

The bottom opening of the box is connected to the ventilation switched on the insufflation mode. Tests performed on the ventilating system as it was switched on the extraction mode assessed that the applicable flow rate is in the range 35 to 320 m³/h.

4.0 MODEL VALIDATION WITH EXPERIMENTAL RESULTS

The comparison of the model with experimental data has been performed in several configurations:

- To verify their consistency, the models were first applied on a case with natural ventilation.
- Using the same configuration as previously but adding mechanical ventilation in a blowing mode, the regime of helium dispersion in the box was observed while making some parameters vary (area of the openings, ventilation rate, height of the release...). The model calculations are compared to the experimental results of the cases leading genuinely to a stratification.
- Due to the scarceness of the tests performed with a ventilation in a blowing mode, the models were also validated against experimental data collected with an extracting ventilation.

4.1 Natural-ventilation test

This special test was realised in the same experimental configuration as the one presented in the next sub-section relative to the mechanically ventilated dispersion tests in a blowing mode. These conditions are summarized in Table 1.

Table 1. Experimental parameters for the natural ventilation test

Nozzle height	Bottom opening	Top opening	Helium release rate	Discharge coefficient
9 cm	Circular shape, diameter 16 cm	Square (12.4 x 12.4 cm)	35 NL/min	0.68

In the adopted configuration, the bottom opening is placed just above the floor, horizontally centered on the vertical wall, while the top opening is located on the roof along the wall facing the bottom opening's one (horizontally centered also). The nozzle used for the release presents a 4 mm-diameter circular shape.

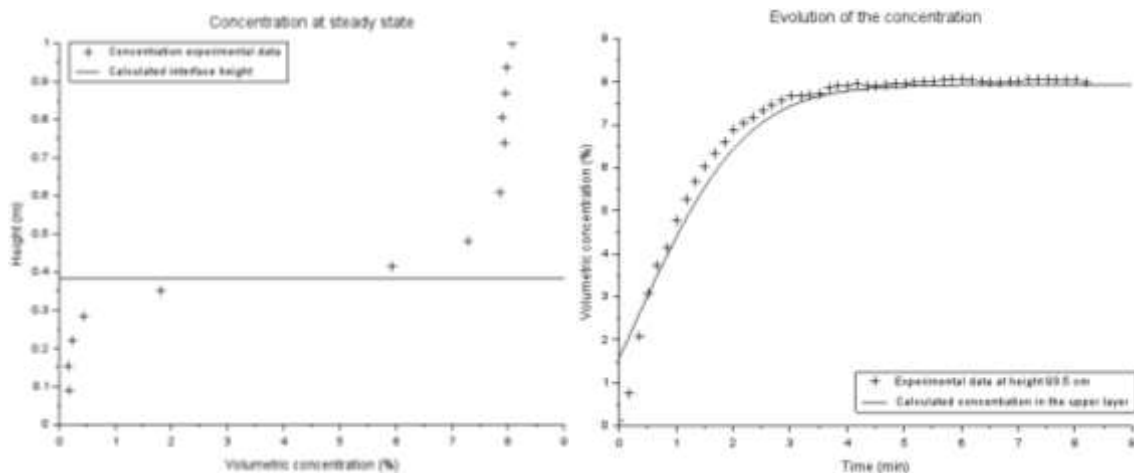


Figure 4. Comparison of the experimental (cross) and analytical (continuous line) results according to the Lowesmith model on a natural ventilation dispersion test (steady state on the left, transitional state on the right)

As can be seen on Figure 4, the Lowesmith model is able to accurately reproduce the experimental data. The stratification in the box at steady state was experimentally obvious and its height was well assessed with this model at 38 cm from the floor, as well as the concentration (7.9 % calculated against 8 %

experimentally). The calculated evolution of the concentration below the ceiling follows also the experimentally observed behaviour, showing a similar duration of the transitional state (around 3 minutes). Concerning the Linden model, the results are not as accurate: the assessed height of the interface is significantly higher (61 cm), as well as the concentration in the upper layer (8.7 %).

4.2 Dispersion tests in a mechanically ventilated enclosure in blowing mode

Among all the tests conducted on the mechanically ventilated box (total amount of 20 tests), making different parameters vary to show their respective influence on the dispersion behaviour of the helium, only 5 of them have led to a stratification. A common point for each of these tests is related to the low level of the ventilation and release flow rates, which is explained as follows:

- High release rates mean that the helium dispersion becomes rather governed by its momentum than its single buoyancy. Consequently, the plume is replaced by a jet, which enhances the homogenisation in the enclosure, either by its collision on the roof and the turbulence it implies. Besides, it makes the model assumptions not valid anymore;
- High ventilation rates experimentally support the homogenisation of the released helium in the enclosure, by disturbing the plume and increasing its velocity.

Table 2. Parameters and experimental/analytical results of the dispersion tests performed on a mechanically ventilated box (insufflation mode)

		Test 1	Test 2	Test 3	Test 4	Test 5
Test conditions	Nozzle height	9 cm	53 cm			
	Bottom opening diameter	16 cm			10.5 cm	
	Ventilation air speed	0.4 m/s			0.75 m/s	
	Top opening side (square)	6.3 cm		12.4 cm	6.3 cm	12.4 cm
Experimental results	Estimated delay to steady state	8 min	4 min	1.5 min	5 min	1.5 min
	Concentration at steady state below the ceiling	13.7 %	17.9 %	10.7 %	17.8 %	10.7 %
	Approximate height of the layer interface	25 cm	65 cm	75 cm	65 cm	80 cm
Linden analytical model	Concentration at steady state in the upper layer	16.3 %	22.9 %	12.7 %	21.3 %	13.0 %
	Height of the layer interface	44 cm	82 cm	94 cm	83 cm	94 cm
Lowesmith analytical results	Estimated delay to steady state	7 min	5 min	2.5 min	6 min	2 min
	Concentration at steady state in the upper layer	11.6 %	12.4 %	9.2 %	14.2 %	9.7 %
	Height of the layer interface	31 cm	73 cm	79 cm	71 cm	78 cm

Table 2 synthesizes the parameters associated with every test kept for the validation, as well as the main estimated experimental and numerical results get. They all have in common the release flow rate (35 NL/min) and the release diameter (4 mm). In each test implying a reduction of the opening area, the opening center is not displaced. Therefore, the circular bottom opening is lifted by a few centimeters.

In this table, the so-called Test 1 corresponds to the same configuration as the one presented in the previous sub-section for which the bottom opening was connected to the ventilation system. The helium release rate as well as the discharge coefficient remain the same as the ones provided in Table 1. All other tests showing a stratification were obtained for a greater height of the release point, at 53 cm rather than 9 cm. Out of the release height, Test 2 corresponds to the same conditions as the reference Test 1, while the conditions of the other tests derive from the ones of Test 2 with various openings areas to show their impact. For both Test 4 and 5, the lower area of the ventilation opening induces a higher inlet air velocity to maintain a constant ventilation power consumption; however, due to important pressure losses associated to the section reduction, the final ventilation rate is lower than for the large bottom opening.

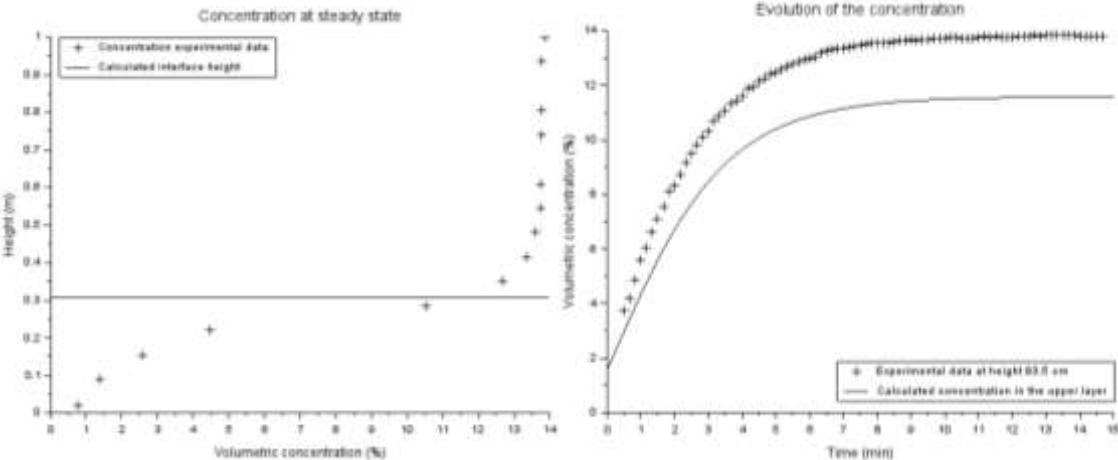


Figure 5. Comparison of the experimental (cross) and analytical (continuous line using the Lowesmith model) results of Test 1 (steady state on the left, transitional state on the right)

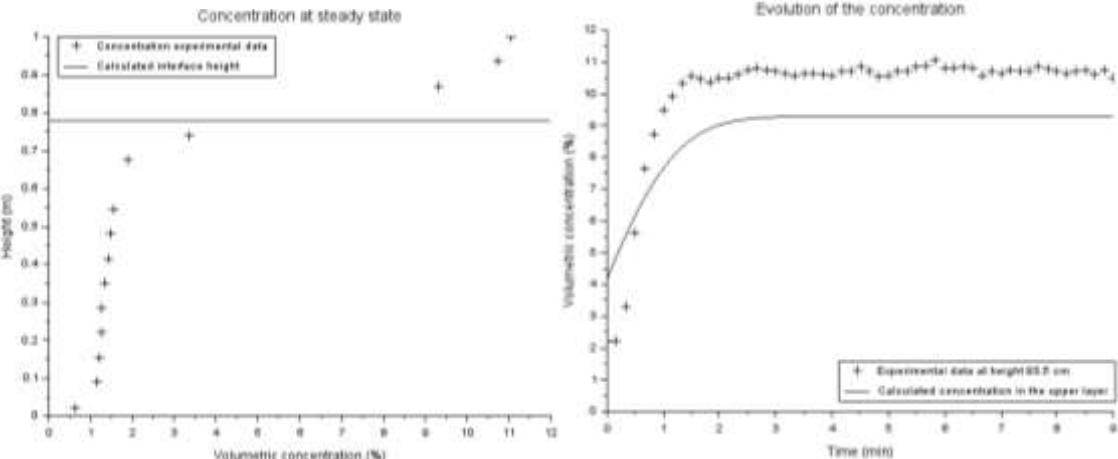


Figure 6. Comparison of the experimental (cross) and analytical (continuous line using the Lowesmith model) results of Test 5 (steady state on the left, transitional state on the right)

Focusing on the results presented in Table 2 as well as on the graphical plots of Figure 5 and Figure 6, it seems that the numerical calculations according to the Lowesmith model do not fit the experimental data as well as it did for the natural ventilation case. This is especially the case regarding the concentration of the upper layer, which is always under-estimated. On the other side, the calculated

height of the layer interface globally matches the height at which the concentration drops genuinely and the behaviour out of the steady state can be quite faithfully reproduced with the Lowesmith model.

Concerning the results of the Linden model, the same observations can be made as in sub-section 4.1: the concentration is in every case over-estimated. However, the model cannot be considered as conservative, as the permanent over-estimation of the interface height reduces the final amount of accumulated light gas in the upper layer and balances this over-estimation (for example for the assessment of the overpressure effects in case of explosion of the mixture).

A potential reason explaining this difference between numerical models and experimental data could be the influence of the ventilation air flow on the plume of released helium. Indeed, this flow is oriented horizontally towards the nozzle and may have, despite its low velocity, disturbed the helium flow. However, this perturbation should not have strongly affected the concentration measurements, as the metal rod carrying the catharometers was placed near a longitudinal wall, parallel to the direction of the ventilation flow and as far as possible from this flux.

4.3 Dispersion tests in a mechanically ventilated enclosure by extraction

As the ventilation by insufflation is rarely applied in practice, the model has also been compared with experimental data collected in the much more common case of ventilation by extraction. This special configuration is besides more commonly used for forced ventilation dispersion tests in the literature [14] [15], which increases the possibilities of comparing the models with experimental data in the future.

Table 3. Experimental parameters for the forced ventilation tests in extraction mode

Nozzle height	Top opening diameter	Bottom opening side	Ventilation air velocity
8 cm	10.5 cm	16 cm	1.4 m/s

Table 4. Experimental/analytical results of the dispersion tests performed on a mechanically ventilated box (extraction mode)

		Test 6	Test 7
Test conditions - Helium release rate		25 NL/min	50 NL/min
Experimental results	Concentration at steady state below the ceiling	4.9 %	9.7 %
	Approximate height of the layer interface	50 cm	50 cm
Linden analytical results	Concentration at steady state in the upper layer	4.1 %	7.9 %
	Height of the layer interface	80 cm	72 cm
Lowesmith analytical results	Concentration at steady state in the upper layer	4.1 %	6.8 %
	Height of the layer interface	50 cm	46 cm

In this proceeding, we focus on the tests performed internally; however, it must be kept in mind that these tests were not realized in the same context than those presented above. This is why the main test conditions, summarized in Table 3, are not exactly the same as in the former sub-section. As previously, the first step consisted in discriminating the tests depending on the generated dispersion regime: two of them, the ones with the lower light gas release rates, led to a stratification with a globally homogeneous helium-enriched upper layer in the box and a downer layer very poor in helium. These both tests were compared with the dispersion models. Note that, despite the change of ventilation mode, no modification has been brought to the modelling: the dimensions and forms of the openings have only been adapted to the test parameters, but the modelling was not changed.

As can be seen in Table 4, both models tend to significantly minimize the concentration of helium in the upper layer. Regarding the height of the upper layer, it seems to be quite well estimated with the Lowesmith model, while the Linden model keeps overestimating it. This shows that these models can poorly be used in such a context and adaptations of the model must be brought beforehand.

It can be noticed that these tests have applied greater air inlet speeds than before. This may have played a role in the discordance of the analytical and experimental results by enhancing the mixing in the enclosure; the agreement between analytical and experimental results could potentially be better with a lower air inlet speed. But such a statement must still be investigated.

5.0 CONCLUSION

Numerical models of wind-assisted light gas dispersion in naturally-ventilated were adapted to the forced ventilation case. To conform to these special conditions, ventilation in an insufflation mode placed near the floor was assumed; such a mode is hardly applied in practice but is the closest one to the conditions for which these models were developed and the most convenient to meet the modelling needs.

The considered models (developed on one side by Linden et al. and on the other by Lowesmith et al.) were restricted to the stratification regime, which means a homogeneous accumulation of the light gas exclusively in an upper layer. To validate this modelling, the models were compared with experimental data collected on a cubic box representing the ventilated enclosure under several conditions: unassisted natural ventilation, blowing mechanically-ventilated enclosure with various parameters and extracting mechanically-ventilated enclosure. It has been noticed that both models show different behaviours:

- The Lowesmith model seems to be very accurate for natural ventilation and likely to reproduce correctly the dispersion for the forced ventilation by insufflation case despite a permanent underestimation of the helium concentration. However, the application in the context of extracting forced ventilation seems to be inadequate without prior adaptation.
- The Linden model seems to be more conservative than the Lowesmith model in terms of concentration of the light gas: it always overestimated this term in both first cases and predicted higher concentrations with the extracting ventilation mode than the Lowesmith model (although being lower than the experimental data). However, it also always overestimates the height of the layer interface, so that it cannot be used to assess the volume of the flammable cloud contained in the enclosure and the overpressure effects of a potential explosion.

For both models, the accuracy of these models is not satisfactory to predict the dispersion in the case of extracting forced ventilation. Further work must be achieved to extend them to such an application.

Beyond these observation, it can be noticed that the test conditions generating a layered dispersion similar to that assumed by the models were restricted to very low ventilation rates. This possibly means that the initial assumption of stratification in the enclosure is not the best-suited one and models based on other premises should be considered or developed. It would be worthwhile to perform large-scale tests to apply larger air inlet speeds; doing so, it would help determining whether the models remain

relevant and applicable for the dispersion in mechanically-ventilated enclosures or must be substituted with more adapted ones.

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