Comparison of two simplified models predictions with experimental measurements for gas release within an enclosure

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ABSTRACT

In this work the validity of simplified mathematical models for predicting dispersion of turbulent buoyant jet or plume within a confined volume is evaluated. In the framework of the HYSAFE Network of Excellence, CEA performed experimental tests in a full-scale Garage facility in order to reproduce accidental gas leakages into an unventilated residential garage. The effects of release velocities, diameters, durations, mass flow rates and flow regimes on the vertical distribution of the gas concentration are investigated. Experimental data confirm the formation, for the release conditions, of an almost well-mixed upper layer and a stratified lower layer. The comparison of the measurements and the model predictions shows that a good agreement is obtained for a relatively longtime gas discharge for jet like or plume like flow behaviour.

Nomenclature

A	Enclosure section [m^2]	V	Enclosure volume [m^3]
B	Buoyancy flux [m^4.s^{-2}]	v	Gas volume [m^3]
D	Diameter [m]	W	Molecular weight [g]
$\mathcal{D}$	mass diffusion coefficient	X	Volume fraction
Fr	Froude number	Y	Mass fraction
g	Gravity acceleration [m.s^{-2}]	z	Vertical coordinate [m]
h	Gas layer thickness [m]	Greek	
H	Enclosure height [m]	α	Taylor entrainment constant
L_{jet}	Characteristic length [m]	μ	Viscosity [Pa.s]
M	Momentum flux [m^4.s^{-2}]	Ω	Overturning ratio
p	Pressure [Pa]	ρ	Density [kg.m^{-3}]
Q	Vertical volume flow rate [m^3.s^{-1}]	Subscripts	
Q'	Entrainment volumetric rate [m^2.s^{-1}]	1	refers to homogeneous layer
Re	Reynolds number	2	refers to stratified layer
Ri	Richardson number	a	refers to free volume air
t	Characteristic time [s]	e	refers to entrainment
U	Velocity [m.s^{-1}]	j	refers to injection

1 Introduction

Safety is a very important issue of the implementation of hydrogen as an energy carrier. The safe use of hydrogen powered vehicles or fuel cell applications in confined spaces would require the ability to predict and mitigate the formation of a flammable accumulation resulting from accidental gas leakage. When the flammable mixture is ignited the overpressure generated may depend on the flammable mass but also on the way hydrogen is distributed. A better knowledge of hydrogen build-up can support accident prevention by determining, for instance, the best location for gas detectors.

In order to reproduce a hydrogen leakage inside a private garage for a single vehicle, a set of experiments have been undertaken at the CEA Garage facility. The experimental data are compared to the predictions of two simplified models. In the tests several mass flow rates and velocities were selected to simulate various possible discharge scenarios.

According to the release conditions and to the enclosure geometry, a potential release can lead to stratified or homogeneous mixed atmosphere. Depending on the ceiling height to floor width aspect ratio, Baines and Turner [1] showed that for narrow enclosures the outflow from the plume turned downward after impinging on the box ceiling and mixed with the ambient. To estimate the degree of overturning they introduce a ratio that compares the destabilising momentum force to the stabilising buoyancy force associated with a plume. This approach has been used to study the mixing process and build-up resulting from natural gas releases by Cleaver et al. [6]. More details about the overturning flow driven by turbulent plume in a cylindrical enclosure have been investigated in a recent study of Kaye and Hunt [7] for a downward discharge. They established that the rise height (layer depth) is a function of the box radius and height when the outflow impinges the sidewall and only on the box height for a pure stratified outflow.

In the case of enclosure with large aspect ratio the fluid reaching the ceiling spreads out and only a stratified layer is produced. Peterson [12] developed a methodology to analyse the mixing behaviour of free and wall jets in large stratified volumes, aimed in particular to study mixing phenomena in nuclear reactor containment.

In the present work, we are interested in small and intermediate-scales momentum releases in a private garage. Two of the existing simplified models addressing the internal dispersion flows are investigated to enable the description of the vertical concentration inside the enclosure. The first model is based on simplified conservation equations and the second on the mass balance in two layers inside the enclosure. According to the flow behaviour (jets or plumes) and to the stability criteria (see Jirka [2]), various leakage starting conditions have been used in order to highlight how the final gas concentration is related to the injection conditions. The remainder of this paper is organised as follow, first we describe the GARAGE facility and the experiments conditions, then jet and plume scaling and the two models are presented. In the last section we compare results of both models with the experimental measurements.

2 Experimental set-up

In order to reproduce realistic hydrogen leakages inside a private garage for a single vehicle, a set of experiments have been undertaken at the so-called CEA Garage facility. The test rig is a rectangular volume representative of a domestic garage (see Figure 1 left). The Garage di-

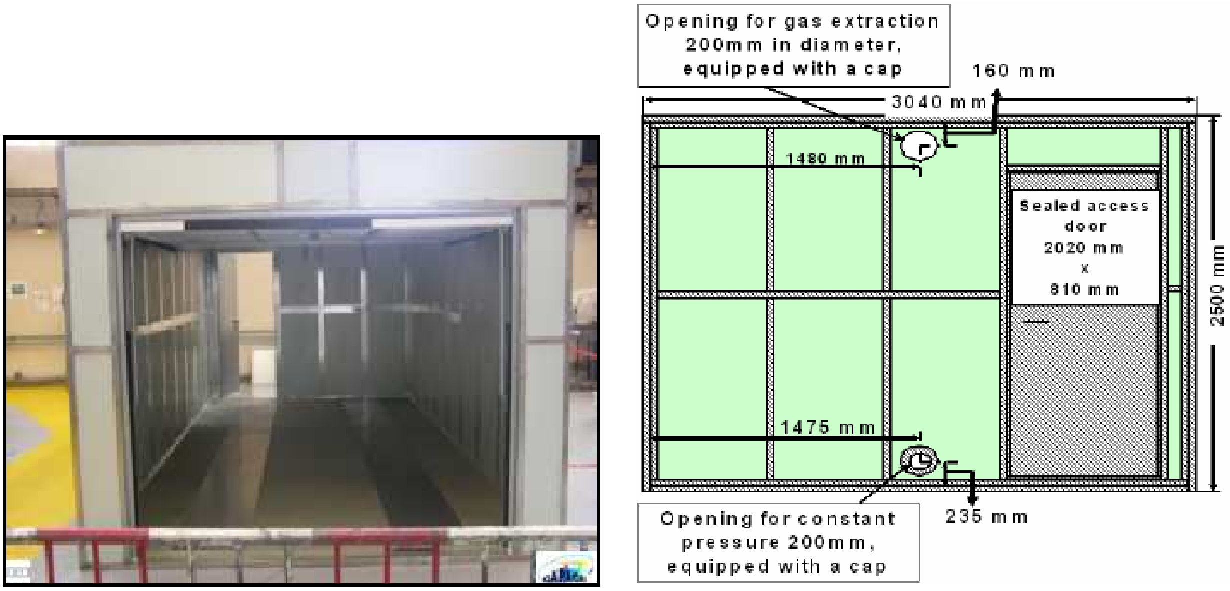

Figure 1: Exterior view of the GARAGE facility at CEA Saclay (left). Rear wall facility (right)

mensions are 5.76m (length)×2.96m (width)×2.42m (height) which gives an internal volume of 40.92 m^3 and a surface section of 16.91 m^2. The Garage is placed inside the experimental hall of the laboratory in order to limit the influence of meteorological conditions. For detailed description of the facility and instrumentation the can refer to [3].
For the sake of safety, dispersion characteristics of hydrogen leakages are simulated with helium. The suitability of helium to simulate the distribution and concentration of hydrogen in a release scenario has been confirmed in previous works such as [13].

2.1 Release conditions

The tests [1–6] consist of pure helium injection phases in a free volume configuration, initially filled with air at atmospheric conditions. The injection phase is then followed by a diffusion phase. The injection, of different durations, is continuous in the upward direction and is located in the middle of the floor ($x_j = 2.88, y_j = 1.48$). A vent is located at ground level, near the back door, opened during the injection phase to avoid the pressurisation of walls. Another vent is located in the upper part of the facility in order to clean up the atmosphere, inside the facility, before the beginning of the experimentation (see Figure 1 right).

2.2 Scaling parameters and volume fluxes modelling

The dimensional analysis allows to determine if the flow discharging from the inlet behaves as a jet or a plume. The Reynolds, Froude and Richardson numbers associated to the injection are given by

$$Re_j = \frac{\rho_j U_j D_j}{\mu_j}, \quad Fr = \frac{\rho_a U_j^2}{g D_j (\rho_a - \rho_j)}, \quad Ri_j = \frac{g D_j (\rho_a - \rho_j)}{2 \rho_j U_j^2}$$

Reference	Test1	Test2	Test3	Test4	Test5	Test6
Mass flow rate (g.s^{-1})	1.99	1.99	0.05	0.2	0.05	0.05
Release duration (s)	120	500	3740	300	400	3740
Injection velocity (m.s^{-1})	35.5	35.5	16.4	3.55	0.46	0.46
Release diameter (mm)	20.7	20.7	29.5	20.7	5	5
Release height (mm)	220	220	220	220	220	220
Reynolds number Re	6277	6277	652.9	627.7	108.8	108.8
Richardson number Ri_j	4.98E-4	4.98E-4	5.64E-4	4.98E-2	4.38	4.38
Richardson number Ri_v	0.16	0.16	0.78	16.59	1005	1005
Froude number Fr	7220	7220	6309	72.20	0.81	0.81
Transition length L_{jet}(mm)	1390	1390	320	139	21	21

Table 1: Releases conditions for the full-scale experiments

In an unconfined environment, the analysis proposed by Chen and Rodi [5] and List [8] gives a definition of a length scale L_{jet} over which the flow has a jet like behaviour.

$$L_{jet} = \frac{3D_j}{2\sqrt{Ri_j}}$$

For a vertically upward jet, L_{jet} is the distance at which the momentum flux produced by buoyancy is comparable to the initial momentum flux.

For Test3, Test4, Test5 and Test6, this length scale is small compared to the distance from the injection to the ceiling, so a plume behaviour can be expected whereas for Test1 and Test2 a jet behaviour is expected.

In the approach proposed by Cleaver et al. [6], a volume Richardson number is introduced to provide some measure of the ability of the jet to promote mixing within the box

$$Ri_v = \frac{\rho_a - \rho_j}{\rho_j}\frac{gV^{1/3}}{U_j^2}$$

On Figure 2, the release conditions of the experiments (Test[1-6]) are compared to the stability criterion established by Jirka [2] for a vertical axisymmetric buoyant jet in shallow water. All experimental data of Figure 2 are in the stable region which supports the assumption of a filling box.

In the following correlations are provided for the entrainment rates and volume fluxes by assuming negligible horizontal gradients of the flow quantities.

2.2.1 Forced jets

For turbulent forced jets List [8] and Peterson [12] propose empirical relations for volumetric entrainment rates

$$Q' = \frac{dQ}{dz} = \frac{Q - Q_j}{H} = \alpha\sqrt{8\pi M} \tag{1}$$

where the Taylor's entrainment coefficient α takes values raging from 0.024 to 0.118 depending on the chosen velocity profile.

By integrating Eq. (1) from the jet source to the ceiling, the volume flow can be written as

$$Q(H_j) = Q_j\left(1 + \alpha 4\sqrt{2}\left(\frac{H_j}{D_j}\right)\right) \tag{2}$$

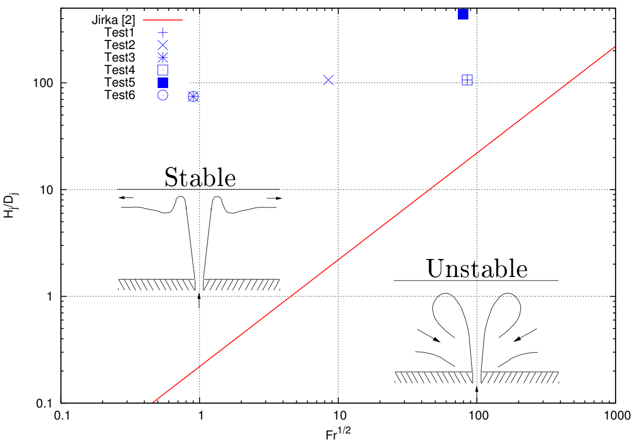

Figure 2: Release conditions compared to the stability criteria for round free buoyant jets [2]

When the buoyancy forces are negligible with respect to the inertia forces, the momentum flux of the jet $M = UQ$ is conserved and is equal to the injection momentum flux

$$\frac{M_j}{M} = \frac{U_j Q_j}{UQ} = \frac{U_j^2 D_j^2}{U^2 D^2} = 1$$

2.2.2 Buoyant plumes

From self-similar turbulent plumes (see List [8]), the dependence of the volume flux Q and the volumetric entrainment rate on the travel distance above the injection source using standard scaling point-source are written as

$$Q(z) = kB^{1/3} z^{5/3} \quad \text{and} \quad Q'(z) = \frac{5}{3} kB^{1/3} z^{2/3} \tag{3}$$

where

$$B = \frac{\rho_a - \rho_j}{\rho_a} g Q_j$$

the constant k is determined by solving the conservation equations for point-source and line plume (see Morton et al. [9]).

$$k = \pi \left(\frac{5}{2\pi\alpha_T} \right)^{1/3} \left(\frac{6\alpha_T}{5} \right)^{5/3}$$

For a buoyant plume with negligible initial momentum (see Cleaver et al. [6]), relationships for the plume radius r and velocity u gave a volume flow depending on the vertical position of

$$Q(z) = 0.079 \left(\frac{\rho_a - \rho_j}{\rho_j} g Q_j \right)^{1/3} z^{5/3} = 0.079 \left(\frac{\rho_a}{\rho_j} \right)^{1/3} B^{1/3} z^{5/3} \tag{4}$$

3 Models description

To describe the mixing of hydrogen into a closed volume with constant cross-section two different simplified models, which are the so-called ambient transport and transient filling box models, are here investigated. Both approaches assume a point source of buoyancy and that the mean velocity in the plume is related to the inflow velocity by the entrainment rate Q'. Furthermore, it is assumed that the density variations are negligible everywhere except in the buoyancy terms.

Following the gas release, the front of buoyant fluid first reaches the upper boundary and begins to descend. The fluid added to the region above the front must have come originally by the entrainment into the plume.

3.1 Model 1: One dimensional ambient transport

This model consists of the simplified conservation equations under stratified conditions resulting from buoyancy forces. The analysis given in [12] shows that the ambient can be considered as stratified for turbulent buoyant jets when the Richardson number based on the entrainment velocity is large compared to the unity and large compared to the inverse of the entrainment Reynolds number. For turbulent buoyant plumes, the criterion of stratification of the ambient is often satisfied when $H_j > L_{jet}$. In these conditions, the concentration distribution can be considered one-dimensional (horizontal gradients are negligible). The conservation equations of the total mass, momentum and species mass fraction are given by

$$\begin{gathered} A(z)\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z}(\rho Q) = -\rho Q' \\ \frac{\partial p}{\partial z} = -\rho g \\ A(z)\frac{\partial \rho Y}{\partial t} + \frac{\partial}{\partial z}\left(\rho Y Q - \rho A(z)\mathcal{D}\frac{\partial Y}{\partial z}\right) = -\rho Y Q' \end{gathered} \tag{5}$$

For a constant cross-section and by neglecting the diffusion and density variations the set of equations reduces to

$$\begin{gathered} \frac{\partial Q}{\partial z} = -Q' \\ A\frac{\partial Y}{\partial t} + Q\frac{\partial Y}{\partial z} = 0. \end{gathered} \tag{6}$$

where Q and Q' are the volume flow and the entrainment rates at z position.

Numerical solution of this set of equations is computed by using a finite difference scheme on a staggered grid for space discretisation and an explicit Euler scheme for time integration. The mass fraction is imposed at the top of the enclosure and is derived from the mass flow rate balance in the enclosure volume.

$$\rho(H)Q(H) = \rho_j Q_j + \int_{z_j}^{H} \rho(z)Q'(z)dz \tag{7}$$

Q is calculated from equations (3) and Q' from equation (1).

The volume fraction is obtained from the following relation

$$X = \frac{\frac{Y}{W_j}}{\frac{Y}{W_j} + \frac{1-Y}{W_a}}$$

In this paper the experimental results are scaled using an entrainment coefficient α of 0.083 which results in a value of $k = 0.15$

3.2 Model 2: Transient model flow in unventilated enclosure

The second model proposed in [6] relies on the identification of two regions in which the following assumptions are made. The upper well-mixed (homogeneous) layer has a constant height h_1 and the lower stratified layer has a time dependent height h_2. The dynamics of mixing are not included in this model.

The rate of change of the gas volume or concentration in each layer is calculated as a function of time and is determined by considering the mass balance in the two layers. So, in a closed region, the downward volume flux in the environment at any level must equal the upward flux in the plume. This leads to the following equations:

$$\frac{\partial v_1}{\partial t} = Q_j + X_2(Q(h_1) - Q(h_1 + h_2)) - X_1 Q(h_1) \tag{8}$$

$$\frac{\partial v_2}{\partial t} = X_1(Q(h_1) - X_2(Q(h_1) - Q(h_1 + h_2)) \tag{9}$$

where v_1 and v_2 are the gas volumes in the upper and the lower layers respectively. The gas concentrations X_1 and X_2 respectively in the upper and the lower layers are determined by

$$X_1 = \frac{v_1}{Ah_1} \quad \text{and} \quad X_2 = \frac{v_2}{Ah_2}.$$

Similarly to the first model, the volume flow rates $Q(h_1)$ and $Q(h_1 + h_2)$ are determined by using equations (2) and (3).

The thickness h_1 is evaluated in the same way as in Cleaver et al. [6]. So, we define the overturning parameter

$$\Omega = \frac{M}{B} = \frac{\pi D \rho u^2}{4A(\rho_a - \rho_j)g}$$

Using the following correlations for r, u and $g\Delta\rho/\rho$ given for a buoyant plume at $z = H_j$

$$D = 0.22z, \quad u = 2.1(g'Q_j/z)^{1/3} \quad \text{and} \quad g\Delta\rho/\rho = 7.1(g'Q_j)^{2/3}/z^{5/3}$$

We obtain that the overturning ratio is function of only geometric parameters $\Omega = 0.215H_j^2/A$ Given the dimensions of the enclosure, Ω is always less than 0.1 for all the cases which gives a well-mixed layer's height $h_1 = 5\Omega H_j$ (see Cleaver et al. [6]). It is noted that the values of Ω is subject to some uncertainty, therefore the values derived above should be considered as indicative only.

The growth in the stratified layer's thickness is given by

$$\frac{\partial h_2}{\partial t} = \frac{Q(h_1 + h_2)}{A} \tag{10}$$

When the stratified layer reach the enclosure bottom ($h_1 + h_2 \geq H$), the equation (9) is replaced by

$$\frac{\partial v_2}{\partial t} = X_1 Q(h_1) - X_2(Q(h_1) - Q_j) \tag{11}$$

and the lower layer depth is fixed to $h_2 = H - h_1$

4 Results and discussions

The experiments, here presented, are selected to assess the models performances for representative cases of vertically upward releases of helium into an enclosure. These cases differ in the flow regime, namely a jet like behaviour for Test1 and Test2, a jet-plume transition for Test3 and Test4 and a plume like behaviour for Test5 and Test6. The jet Reynolds number values ranging from Re = 108 to 6277 cover the laminar-turbulent transition and the fully turbulent regime. The measurement uncertainties for experiments are around 0.1%. In Figures [3 – 8], the curves with symbols illustrate the experimental data of the concentration distribution expressed as a percentage of the average concentration (volume fraction) value at any elevation. Curves without symbols represent the models predictions. The comparisons for each test are made at different intermediate time steps.

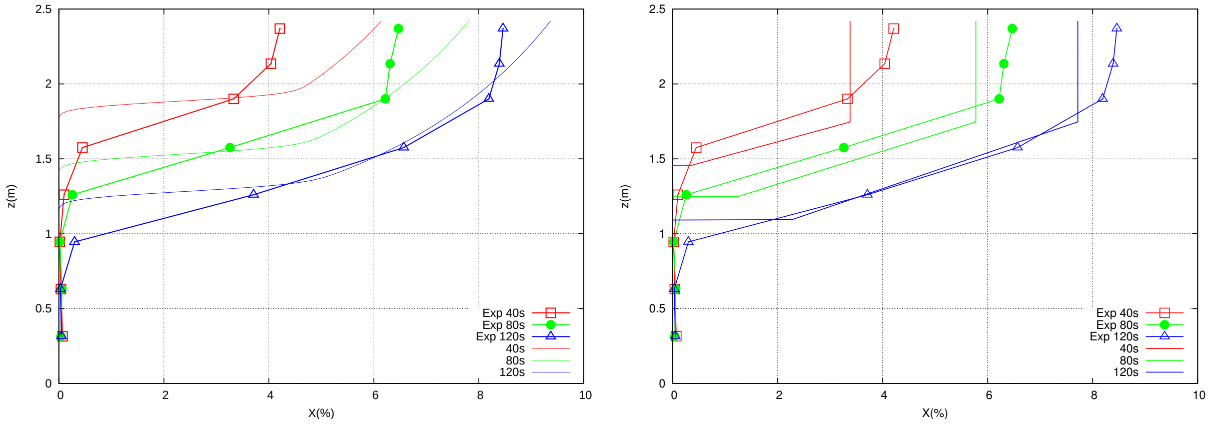

Figure 3: Test1: Vertical profiles of helium concentrations. Comparison of experimental data with predictions of: model1 (left), model2 (right)

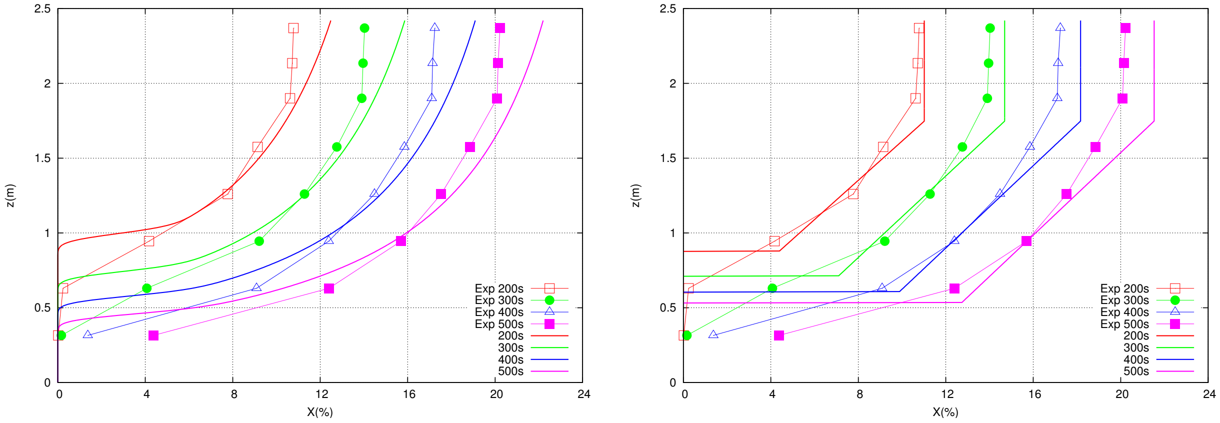

Figure 4: Test2: Vertical profiles of helium concentrations. Comparison of experimental data with predictions of: model1 (left), model2 (right)

In the cases Test1 and Test2 shown in Figures 3 and 4 the flow with relatively high velocity release behaves as a jet. At earlier times $t = 40s, 80s$ (see Figure 3), significant discrepancies from measurements are noticeable for both models more particularly for model1. Later on

($t > 100s$), a rather good agreement with experiments is obtained for the two models even if the maximum concentration is slightly overestimated as shown in Figure 4. This is confirmed by the corresponding time evolutions shown on Figure 9. For longtime discharge one can see from measurements (Figure 4) that the Test2 tends to produce more well-mixed upper layer with an almost uniform concentration.

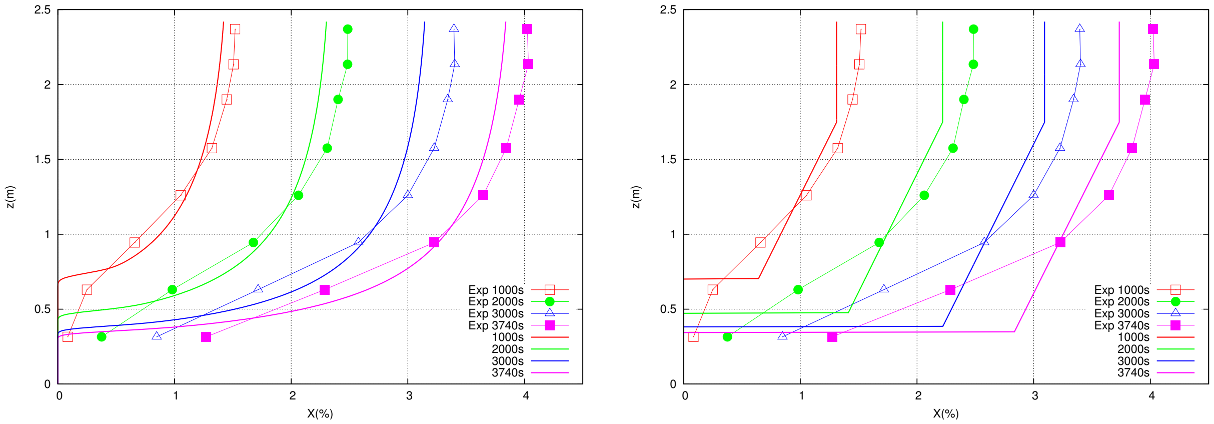

Figure 5: Test3: Vertical profiles of helium concentrations. Comparison of experimental data with predictions of: model1 (left), model2 (right)

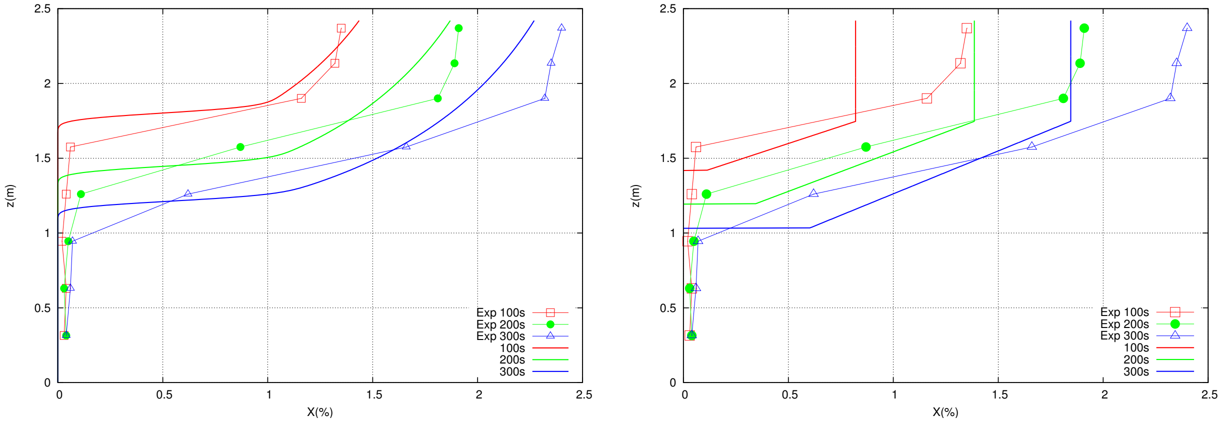

Figure 6: Test4: Vertical profiles of helium concentrations. Comparison of experimental data with predictions of: model1 (left), model2 (right)

Results of Test3 and Test4 for jet-plume transition flows with small discharge flow rates (in Figures 5 and 6) show that both models give smaller values of concentration in the upper part of the volume and larger concentrations below. Comparisons in Figure 6 of the Test4, carried out for brief time release, show that the models clearly underestimate the maximum concentrations for earlier times. Figure 10 shows that the average concentration from models, although being consistent with the specified injection mass, is lower than the average of measured concentrations.

In Test5 and Test6 cases, the flow is dominated by buoyancy forces. Brief and longtime releases are presented. Figure 7 shows that models provide better agreement for concentration distribution at small times compared to the jet and the jet-to-plume transition cases. This

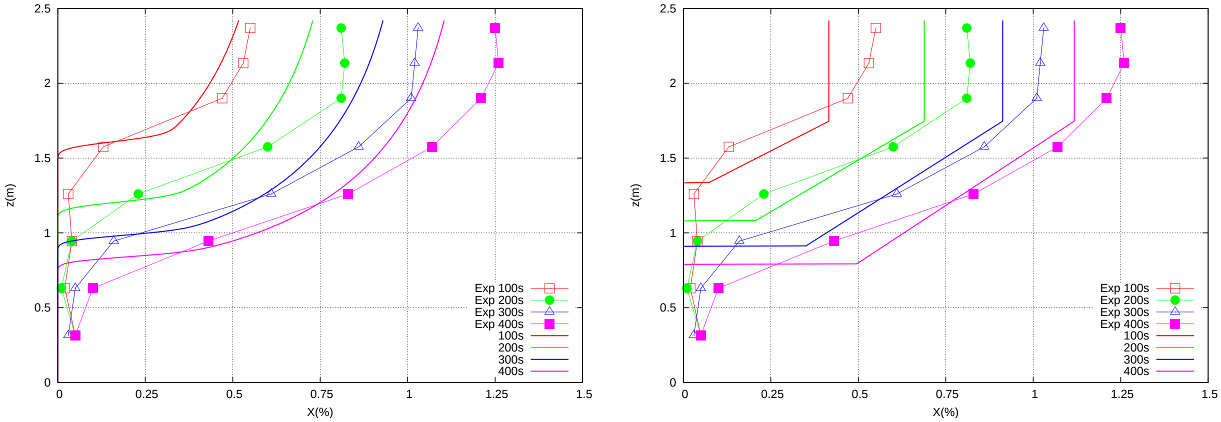

Figure 7: Test5: Vertical profiles of helium concentrations. Comparison of experimental data with predictions of: model1 (left), model2 (right)

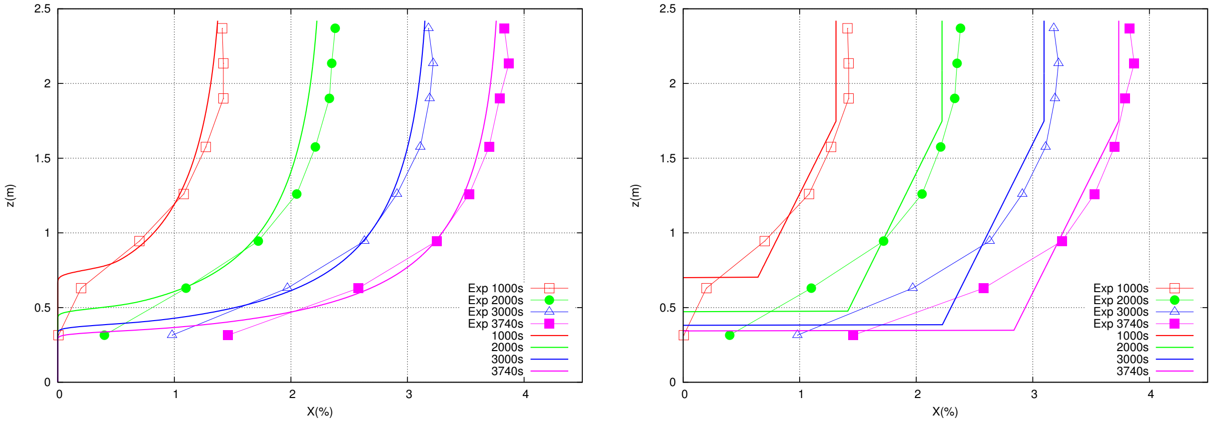

Figure 8: Test6: Vertical profiles of helium concentrations. Comparison of experimental data with predictions of: model1 (left), model2 (right)

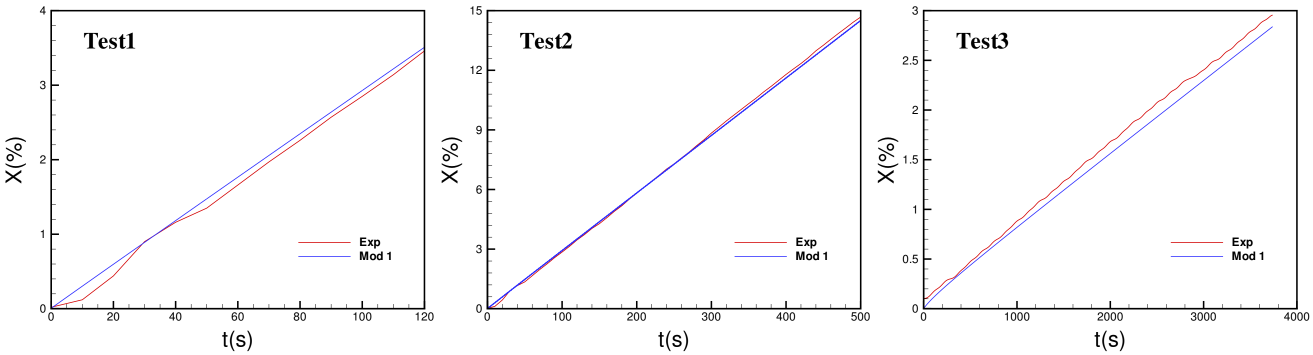

Figure 9: Comparisons of the time evolutions of the averaged concentrations for brief time discharges

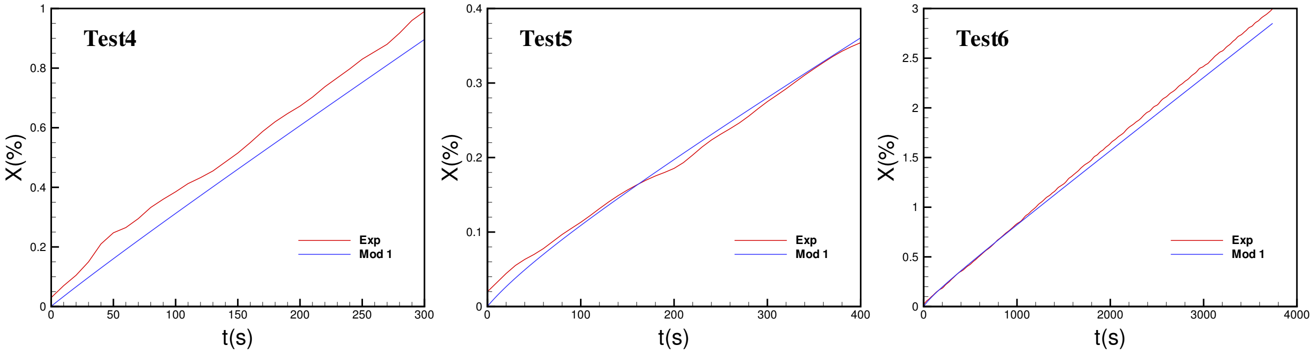

Figure 10: Comparisons of the model1 predictions with the experimental data for the time evolutions of the averaged concentrations for lontgime discharges

can be also observed on the the temporal evolution of the averaged concentration (see Figure 10). For longtime discharge, agreement between the models results and the measurements is clearly increased but the upper layer concentrations are faintly underestimated (see also Figure 10). More correct description is here obtained for the growth of the lower stratified layer. These results could be justified by the use of plume correlations to estimate the flow rate.

It should be mentioned that the comparison between the two models predictions show that results fit fairly well with each other except for Test1 and Test4.

5 Conclusions

A series of experiments have been conducted to verify the capabilities of two simplified models for a jet, a jet-plume and a plume like flows generated by helium releases within an enclosure. The experimental tests concern vertical upward releases with leakage starting conditions leading to stable stratification.

Within the limitations of the simplified models, the overall features of the concentration distribution and mixture accumulation are captured. Indeed, the experiments confirm the stratification of the gas mixture within the volume irrespective to the leakage mass flow rate. A thick upper layer of nearly uniform concentration is formed.

The models predictions provide reasonable comparisons of the vertical concentration profiles with experimental measurements. Good agreement is obtained for long duration releases in particular for buoyant plumes with small mass flow discharge. Even if the correlations used to estimate the volume flow rates are scaled for buoyant plumes, good description is provided for jets which shows that these models are also well adapted for jets.

Both models are not appropriate to describe concentration distribution for brief time gas discharge. This is in part due to the assumption of free horizontal gradients of the flow quantities adopted in both models.

Development work could be undertaken to estimate concentration for releases in which overturning may occur and to consider horizontal and downward leakages.

References

[1] Baines, W. D. and Turner, J. S., Turbulent buoyant convection from a source in a confined region. *Journal of Fluid Mechanics*, 37, 1969, pp.51-80.

[2] Jirka, G. H., Turbulent buoyant jets in shallow fluid layers, In: *Turbulent Buoyant Jets and Plumes* (edited by W. Rodi). 1982. Pergamon Press, New York.

[3] Gupta, S., Brinster, J., Studer, E. and Tkatschenko, I. Hydrogen related risks within a private garage: Concentration measurements in a realistic full scale experimental facility, International conference on hydrogen safety, 2006.

[4] Houf, W. and Schefer, R., Small-scale unintended releases of hydrogen, In *Annual Hydrogen Conference and Hydrogen expo USA, March 19-22, 2007, San-Antonio TX.*

[5] Chen, C. J. and Rodi, W., A review of experimental data: vertical turbulent buoyant jets. 1980. Pergamon Press, Oxford.

[6] Cleaver, R. P., Marshall, M. R. and Linden P. F., The build up of concentration within a single enclosed volume following a release of natural gas. *Journal of Hazardous Materials*, 36, 1994, pp.209 ŋ 226.

[7] Kaye, N. B. and Hunt, G. R., Overturning filling box, *Journal of Fluid Mechanics*, 576, 2007, pp. 297-323.

[8] List, E. J., Turbulent jets and plumes, in: Fisher, H. B., List, E. J., Koh, R. C. Y., Imberger, J. and Brooks, N. H. (Eds.), Mixing in Inland and Coastal Waters. Academic Press, New York, 1979, Ch. 9, pp. 315-389.

[9] Morton, B. R., Taylor, G. I. and Turner, J. S., Turbulent gravitational convection from maintained and instantaneous sources. *Proc. R. Soc. Lond.* A 234, 1-23.

[10] Birch, A. D., Brown, D. R., Dodson, M. G. and Swaffield, F., The structure and concentration decay of high pressure jets of natural gas, *Combustion Science and Technology*, 36, 1984, pp. 249-261.

[11] Schefer, R. W., Houf, W. G. and Williams, T. C., Investigation of small-scale unintended releases of hydrogen: Buoyancy effect, *International journal of hydrogen energy*, 33, 2008, pp. 4702-4712.

[12] Peterson, P. F. Scaling and analysis of mixing in large stratified volumes, *International journal of heat and mass transfer*, 37, 1994, pp. 97-106.

[13] Swain, M. R., Filoso, P., Grilliot E. S. and Swain M. N.,. Hydrogen leakage into simple geometries enclosures. *International journal of hydrogen energy*, 28, 2003, pp. 229-248.