Estimation Of An Allowable Hydrogen Permeation Rate From Road Vehicle Compressed Gaseous Hydrogen Storage Systems In Typical Garages; Part 2: CFD dispersion calculations using the ADREA-HF code and experimental validation using helium tests at the GARAGE facility

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Abstract

The time and space evolution of the distribution of hydrogen in confined settings was investigated computationally and experimentally for permeation from typical compressed gaseous hydrogen storage systems for buses or cars. The work was performed within the framework of the InsHyde internal project of the HySafe NoE, funded by EC. The main goal was to examine whether hydrogen is distributed homogeneously within a garage like facility or whether stratified conditions are developed, under certain conditions. The nominal hydrogen flow rate considered was 1.087 NL/min, based on the then current SAE standard for composite hydrogen containers with a non-metallic liner (type 4) at simulated end of life and maximum material temperature in a bus facility with a volume of 681m^3. The release was assumed to be directed upwards from a 0.15m diameter hole located at the middle part of the bus cylinders casing. Ventilation rates up to 0.03 ACH were considered. Simulated time periods extended up to 20 days. The CFD simulations performed with the ADREA-HF code showed that fully homogeneous conditions exist for low ventilation rates, while stratified conditions prevail for higher ventilation rates. Regarding flow structure it was found that the vertical concentration profiles can be considered as the superposition of the concentration at the floor (driven by laminar diffusion) plus a concentration difference between floor and ceiling (driven by buoyancy forces). In all cases considered this concentration difference was found to be less than 0.5%. The dispersion experiments were performed at the GARAGE facility, using Helium. Comparison between CFD simulations and experiments showed that the predicted concentrations were in good agreement with the experimental data. Finally, simulations were performed using two integral models: the fully homogeneous model and the two-layer model, proposed by Lowesmith et al. (ICHS-2, 2007) and the results were compared both against CFD and the experimental data.

1 INTRODUCTION

In the past [1] the problem of the accumulation of hydrogen in confined spaces due to permeation has been analyzed using the simple homogeneous model, described in section 3.2. The model assumes that the released gas is homogeneously distributed within the free volume of the facility. Hydrogen buoyancy on the other hand creates stratification as the lighter fluid is accumulated closer to the ceiling. Stratification leads to higher concentrations2 and therefore the time to reach the lower flammability limit (LFL) can be shorter than what is predicted by the homogeneous model.

The aim of the present work was to investigate using a validated CFD code whether homogeneous or stratified conditions develop within the garage-like facility where hydrogen is assumed to be released by permeation from a typical automotive storage system and thus test the applicability of the homogeneous model approach in the case of permeation.

The work was performed within the framework of the InsHyde internal project of the HySafe NoE, co-funded by EC, which the authors gratefully acknowledge. The present paper represents part 2 of the work, see [3].

2 SCENARIOS

Four scenarios were examined in total. Table 1 presents a general overview. The first two scenarios consider a CGH2 bus horizontally centred inside a single bus maintenance facility, see Figure 1. Bus dimensions were 12x2.55x3.0 m in length, width and height. Distance between bus and floor was taken as 0.4m. Hydrogen was assumed to be released vertically upwards from a 0.15m diameter hole located at the centre of the cover over the roof mounted hydrogen containers (at z=3.5 m). The hydrogen release rate was calculated at 1.087 NL/min, based on the then current SAE (Society of Automotive Engineers) standard for composite hydrogen containers with a non-metallic liner (type 4) at simulated end of life (EoL) and at maximum material temperature conditions (MMT), see [4]. More specifically, SAE had proposed a max allowable value of 75 NL/min for a 47 m^3 private car garage. The current value was obtained by multiplying the SAE value by the garage volume ratio (681 / 47 = 14.5), to account for the difference in facility volume between private car and bus. Table 2 presents the source conditions in detail.

The first two scenarios are distinguished based on the assumed ventilation rate. In Bus-2 scenario a value of 0.03 ACH was assumed. This value was identified in [3] as a "reasonable minimum value", based on an analysis of a series of measurements, including the ventilation rate measurements performed by CEA within the present study. For Bus-1 scenario the air exchange rate was selected as an order of magnitude lower than in Bus-2, i.e. 0.001 ACH.

The next two scenarios (CEA-1 and 2) were analyzed both computationally (CFD) and experimentally. Tests were performed by CEA at the GARAGE facility without any vehicle inside, using helium (instead of hydrogen for safety reasons) released vertically upwards from a hole located at the centre of the floor. The GARAGE facility was thought as roughly representing the empty space between the bus top and the bus-garage ceiling. In both cases the ventilation rate was assumed 0.01 ACH, which was the minimum value identified by CEA in separate ventilation tests with helium. The CEA scenarios differ with respect to the permeation flow rate. A value of 1 NL/min i.e. similar to scenarios Bus-1 and 2 was employed for CEA-1. For CEA-2 the experiments were performed using the minimum available flow rate (0.03 L/min).

Finally it should be noted that in all the simulated cases the air change rate (ACH) was externally imposed, rather than being left free to develop as a result of the released gas for given openings. Two openings were assumed present in each case. A fresh air inlet opening assumed located at the bottom centre of one of the two shortest walls and a top opening located at the centre of the ceiling. The ACH rate for fixed facility geometry was varied by varying the inflow/outflow velocity. The assumed ventilation rate, dimensions of the openings and inflow/outflow velocities are presented in Table 3.

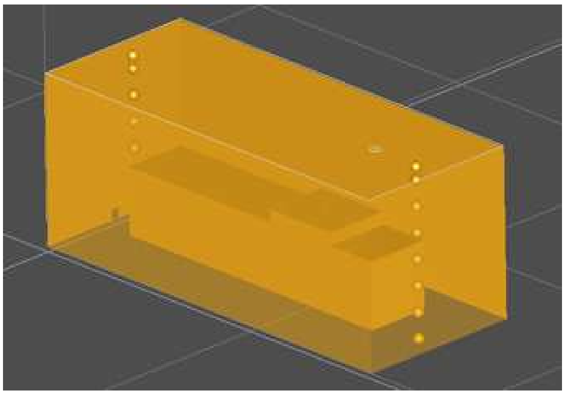


Figure 1 Facility for bus scenarios

Table 1 Scenarios overview: ^{A} SAE proposal at end of life (EoL) and maximum material temperature (MMT) for type 4 cylinders, ^{B} Free volume assumed 597.8 m3, ^{C} Normal conditions are 20 °C and 1 atm (101325 Pa)

Scenario	Facility dimensions (m) (length x width x height)	Release rate (NL/min)^C	Released substance	Ventilation rate (ACH)
Bus-1	16 x 6.55 x 6.0 (681.2 m3)^B	1.087^A	H2	0.001
Bus-2	16 x 6.55 x 6.0 (681.2 m3) ^{B}	1.087 ^{A}	H2	0.03
CEA-1	5.76 x 2.96 x 2.4 (40.92 m3)	1.0	He	0.01
CEA-2	5.76 x 2.96 x 2.4 (40.92 m3)	0.03	He	0.01

Table 2 Source conditions

Scenario	Exit Diameter (m)	Exit Velocity (10-3 m/s)	(H2 or He) Concentration
Bus-1	0.15	1.07	1.0
Bus-2	0.15	1.07	1.0
CEA-1	0.07	4.33	1.0
CEA-2	0.07	0.13	1.0

Table 3 Ventilation conditions

Scenario	Inlet area (m2)	Inlet velocity (10-3 m/s)	Outlet area (m2)	Outlet velocity (10-3 m/s)
Bus-1	0.22	0.75	0.12	1.5
Bus-2	0.22	22.4	0.12	41.7
CEA-1	0.01	11.37	0.01	13.03
CEA-2	0.01	11.37	0.01	11.42

3 COMPUTATIONAL METHODOLOGY

3.1 CFD calculations with the ADREA-HF code

The CFD calculations were performed using the ADREA-HF code earlier validated for hydrogen [5, 6, 7] and helium [8] dispersion within confined spaces. The code solves the 3d transient fully compressible conservation equations for mixture mass, mixture momentum, mixture energy and species mass. In the present simulations working fluid was a mixture of dry air plus hydrogen (or helium for CEA tests). The energy equation was not used and conditions were assumed isothermal. Turbulence was modelled using the standard k-epsilon model [9], extended for buoyant flows.

In all cases simulated the computational domain was fitted to the facility and symmetry was not assumed. The computational grid was Cartesian and non-equidistant. For the bus scenarios the grid consists of 36x23x32 (26496) grid cells in X, Y and Z directions (length, width, height). The minimum cell is located at the source and has size 0.15 m. For the CEA scenarios the grid consists of 27x19x25=12825 grid cells in X, Y and Z directions (length, width, height). The minimum cell is located at the source and has size 0.1 m. The horizontal expansion ratio was 1.12 in all cases.

Dirichlet (i.e. given value) boundary conditions were used for the normal flow velocity at the two openings. Normal velocity values were as given in Table 3. It is noted that in this table the fresh air inlet velocity was calculated based on the assumed ACH, while the outflow velocity by assuming that at every instant of time the outflow (m3/s) through the facility equals the inflow of fresh air and released gas.

Finally, the first order upwind scheme was used for spatial discretization. The first order Euler fully implicit scheme was used for temporal discretization. The maximum time step size was restricted by setting a max convective CFL number of 5.

3.2 The homogeneous model

In the homogeneous model, see section 10.20 of Lees, (1996) [10], the released gas is assumed homogeneously distributed within the free space of the enclosure. The enclosure is assumed to have two openings, a fresh air inflow opening and an outflow opening for the mixture of air plus released gas. The gas concentration is obtained from the following gas mass conservation equation:

$$V\frac{dc}{dt} = Q_s - c\left(Q_s + Q_{in}\right) \qquad [1]$$

V is the free-volume of the facility which is assumed constant over time, Q_S is the source volumetric flow rate, Q_{in} is the volumetric flow rate of the fresh air entering the facility, t is the time and c is the molar concentration (v/v).

The above equation can be solved analytically to give:

$$\mathrm{c} = \frac{Q_s}{Q_s + Q_{in}}\left(1 - \exp(-\frac{Q_s + Q_{in}}{V}t)\right) \qquad [2]$$

In the special case of a fully closed box (referred below as “0 ACH” case) the concentration is calculated from:

$$V\frac{dc}{dt} = Q_s \Rightarrow c = \frac{Q_s t}{V} \qquad [3]$$

3.3 The two-layer model

The gas build-up in a domestic property following releases of methane/hydrogen mixtures has been investigated by Lowesmith et al. (2007) [11]. Experiments were performed and a two-layer model was developed and validated using the performed tests. Figure 2 shows the assumed geometry.

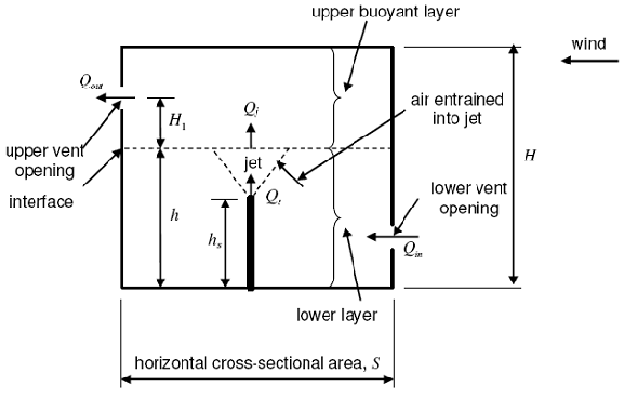


Figure 2 Geometrical configuration for the two-layer model, taken from Lowesmith et al. (2007)

The released substance is assumed homogeneously distributed within the upper layer, which has a height varying with time. The concentration of the released substance in the upper layer and the upper layer volume are obtained from the conservation equations of mixture mass and released gas mass as given below:

$$\frac{dV_{up}}{dt}=Q_j-\left(Q_s+Q_{in}\right),\quad V_{up}\frac{dc}{dt}=Q_s-c\left(Q_s+Q_{in}\right) \qquad [4]$$

V_{up} is the upper layer volume, which is a function of time and c is the molar concentration (v/v) in the upper layer. Q_j is the volumetric flow rate of air-gas mixture passing through the plume cross sectional area at the level of the interface (z = h). To obtain Q_j the axi-symmetric horizontally integrated plume equations for mixture mass, momentum and hydrogen mass conservation given below are vertically integrated from the level of the source up to the level of the interface.

$$\frac{dWR^2}{dz}=2R\alpha W,\quad \frac{dW^2R^2}{dz}=g'(\lambda R)^2,\quad g'=g\frac{\rho_a-\rho_j}{\rho_a},\quad \frac{dg'WR^2}{dz}=0 \qquad [5]$$

In the above equations W is the plume velocity, z is the vertical distance from source, R is the local plume radius, α = 0.05 is the entrainment coefficient and λ = 1.1 is the ratio of horizontal to vertical length scales.

A computer program was prepared to solve the above equations and obtain the level of the interface and the upper layer concentration as function of time. The fresh air inflow was externally imposed (i.e. given ACH) rather than calculated as described in Lowesmith et al. (2007).

4 EXPERIMENTAL METHODOLOGY

Experiments have been conducted on the GARAGE facility. This is a full scale parallelepiped enclosure of 5.76m long, 2.96m wide and 2.42m high with a typical garage tilting door of 2.32m wide by 1.99m high on the front and a classical door of 0.81m wide by 2.02m high on the back for human access. Two vents are located in the middle of the back wall near the floor and near the ceiling. Helium is used as a model gas for hydrogen. It is injected in the enclosure through a vertical nozzle of 70mm in diameter centred in the enclosure at 210mm from the floor. A mass flow rate regulator is used for the injection of 0.030±0.001Nl/min and 1.000±0.006Nl/min.

The local volume concentration is measured with mini-catharometers TCG-3880 from Xensor. 30 sensors are distributed in the enclosure along 6 vertical lines at 5 levels (0.2m, 0.7m, 1.2m, 1.7m and 2.2m from the floor). Temperature is measured with thermocouples at 10 locations near the floor and near the ceiling.

The lowest leak rate of the enclosure is obtained by obstructing the tilting door and sealing the back door with aluminium tape. Both vents are closed. The ACH of the enclosure in this configuration has been measured with the tracer gas decay method which gives 0.01h^{-1}.

5 RESULTS AND DISCUSSION

5.1 Two-layer model evaluation

Figure 3 (left) shows a comparison between concentration histories predicted with the two-layer model and the fully homogeneous model, for various ACH. Figure 3 (right) shows the corresponding predicted interface elevations for two-layer model. It can be observed that the two-layer model gives significantly higher concentrations compared to the homogeneous model and also arrival times to given concentration significantly lower than in the homogeneous model. The reason for this behaviour is the level of the interface, which as shown in Figure 3 is for the two-layer model never below the source position (assumed at 3.5m).

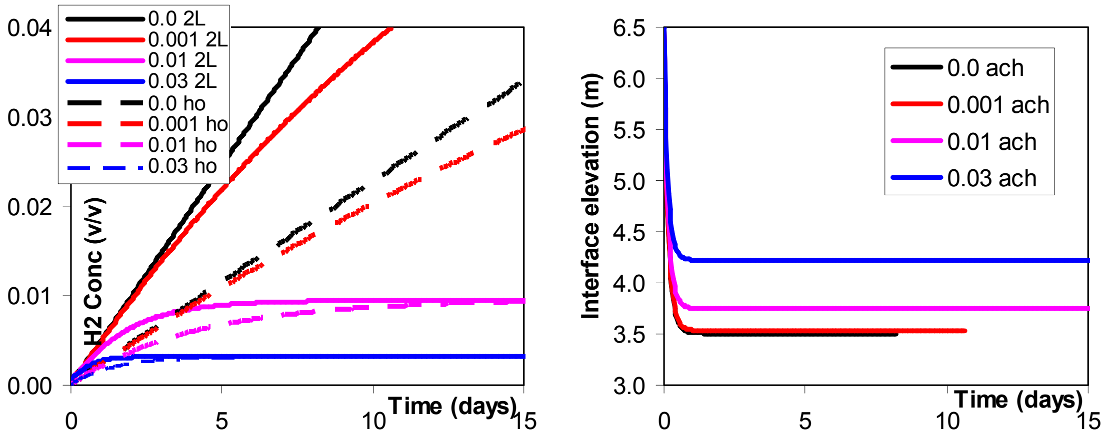


Figure 3 Bus scenarios: Left: Predicted concentration history with two-layer model (2L) compared with fully homogeneous model (ho) for various ACH, Right: Predicted interface elevation with two-layer model for various ACH

5.2 Scenario bus-1

CFD simulations for scenario Bus-1 were performed for a release period of 20 days. According to the homogenous model the time at which concentration becomes greater than hydrogen LFL (4%) is approximately 15.2 days for 0 ACH and 19.6 days 0.001 ACH. Figure 4 (top) shows the predicted concentration time series at various heights from near floor to near ceiling. The shown horizontal location of the sensors is not important, since CFD solution shows large horizontal homogeneity. The CFD solution is compared against the homogeneous model mentioned above. It is observed that CFD predicts 18.8 days for the concentration to become greater than LFL at 5m from floor, i.e. approximately 1 day earlier than the homogenous model with 0.001 ACH. The predicted vertical concentration profiles at various times after start of release are shown in Figure 4 (bottom-left). It is observed that although the concentrations levels are gradually increasing the structure of the concentration profile remains nearly constant with time, with a concentration difference between bottom and ceiling of approximately 0.5%. Figure 4 (bottom-right) shows the predicted hydrogen mass inside the facility. It is observed that the CFD model accurately coincides with the results of the homogeneous model with the same ACH.

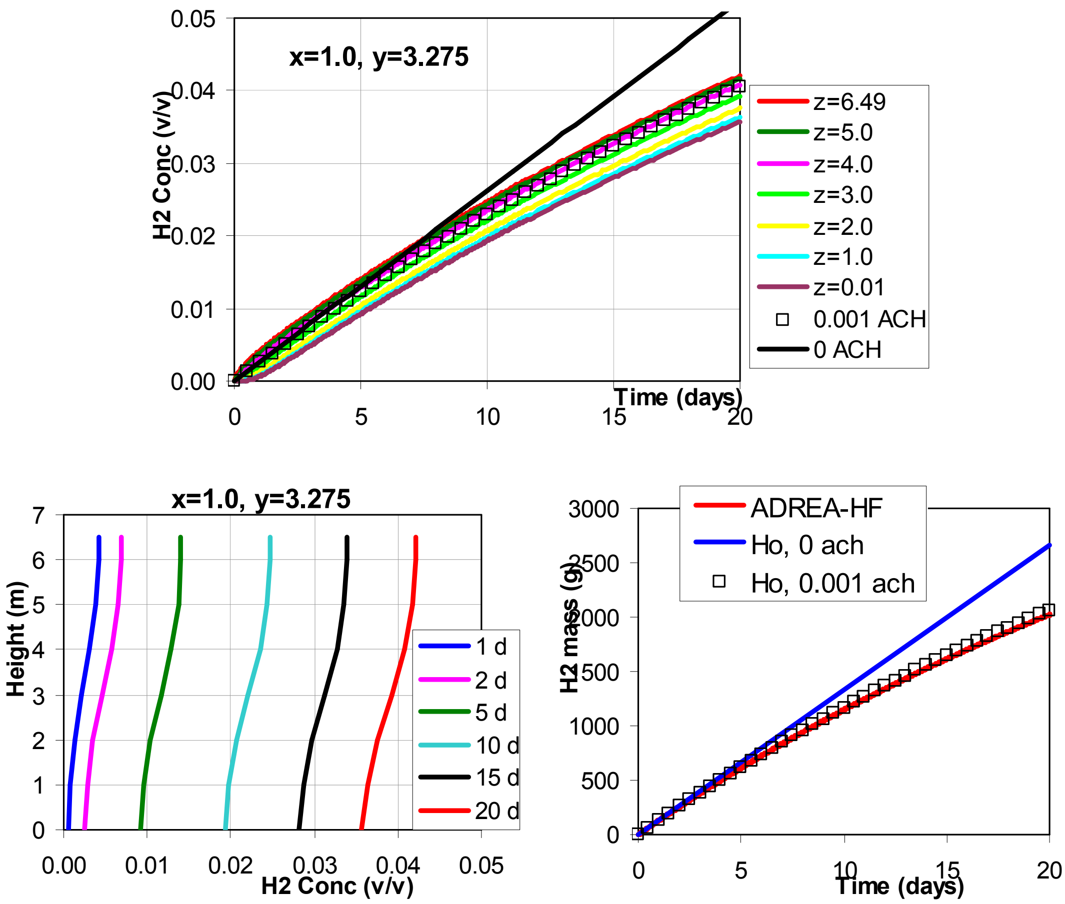


Figure 4 Scenario Bus-1: Top: CFD predicted concentration histories at various heights compared against homogeneous model (black line and boxes). Bottom left: CFD predicted vertical concentration profiles at various times from start of release in days. Bottom right: CFD predicted hydrogen mass inside the facility compared against homogeneous model (Open boxes and blue line).

5.3 Scenario bus-2

CFD simulations for scenario Bus-1 were performed for a release period of 5 days. CFD simulations and homogeneous model with 0.03 ACH showed that at this time steady state conditions were approached. Figure 5 (top) shows the predicted concentration time series at various heights from near floor to near ceiling. CFD solution is compared against the homogeneous model. The predicted vertical concentration profiles at various times after start of release are shown in Figure 5 (bottom left). It is observed that the maximum concentration difference between ceiling and floor is approximately 0.4%, i.e. nearly same as in Bus-1. Figure 5 (bottom right) shows the predicted hydrogen mass inside the facility. It is observed that the CFD model prediction departs from the homogeneous model prediction with the same ACH, in contrast to what was observed in case bus-1.

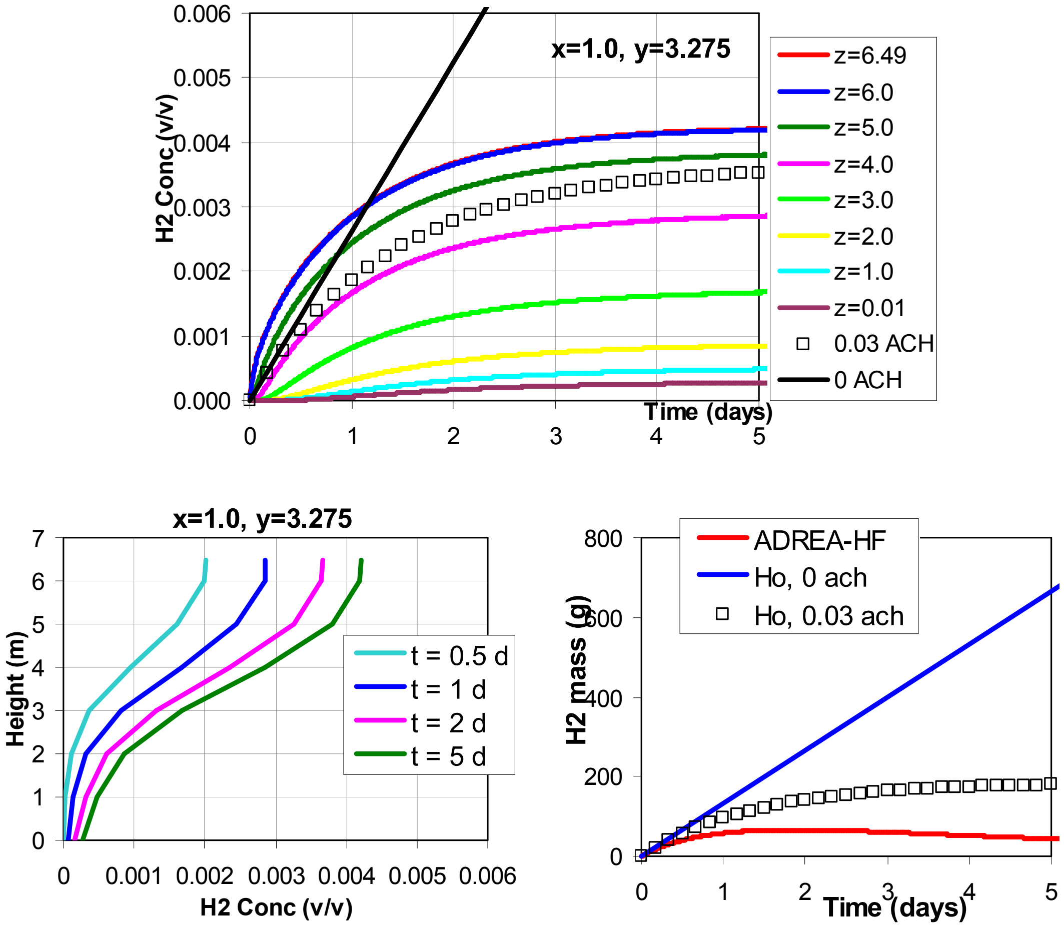


Figure 5 Scenario Bus-2: Caption as in Figure 4.

5.4 Scenario CEA-1

CEA-1 helium dispersion experiments were performed for a release period of 2.3 days. Figure 6 shows a comparison between measured and predicted helium concentration for a period of approximately 8.3 hours. Figure 7 shows the same comparison for a period of 2.3 days. Agreement between CFD, homogeneous model and experimental data is quite satisfactory. Both give a 0.2% max concentration difference between ceiling and floor, which is near the corresponding values for Bus-1 and 2, for approximately the same flow rate. It should be noted that a homogenization and subsequent stratification phenomenon was observed in the experiments as shown in Figure 7. This is related to non-fully isothermal conditions holding during the tests, more specifically an inversion in the temperature gradient in the enclosure. CEA observed a weak (between 0.1°C and 0.2°C) stable temperature gradient when concentration stratification is observed, while the temperature is homogeneous or slightly inverted when the concentration is homogenous.

The CFD simulation was continued for a total release period of 10 days and Figure 8 (top) shows the predicted concentration time series at various heights from near floor to near ceiling. CFD solution is compared against the homogeneous model. The predicted vertical concentration profiles at various times after start of release are shown in Figure 8 (bottom left). It is observed that the structure of the concentration profile remains nearly constant with time. Figure 8 (bottom right) shows the predicted helium mass inside the facility. It is observed that the CFD model accurately predicts the results of the homogeneous model with the same ACH.

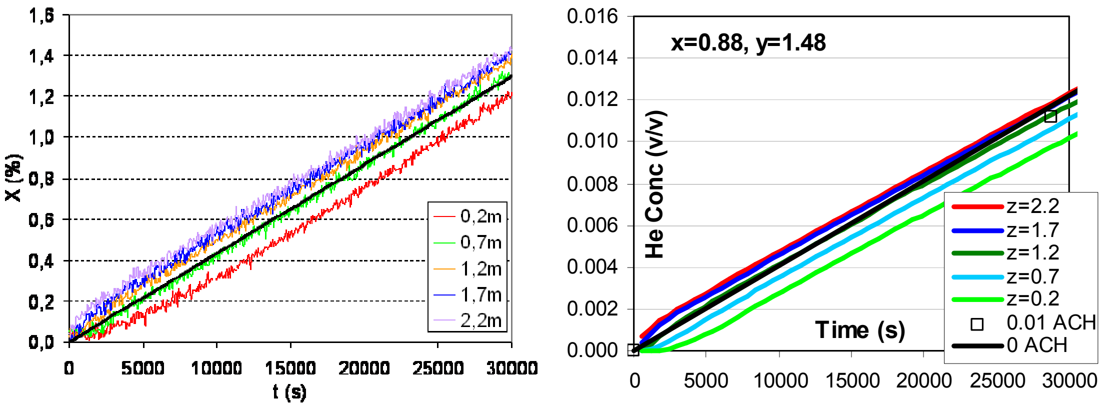


Figure 6 CEA-1: Comparison between measured (left) and predicted (right) concentration time series for a period of approximately 8.3 hours. Open boxes and black line show the homogeneous model solutions

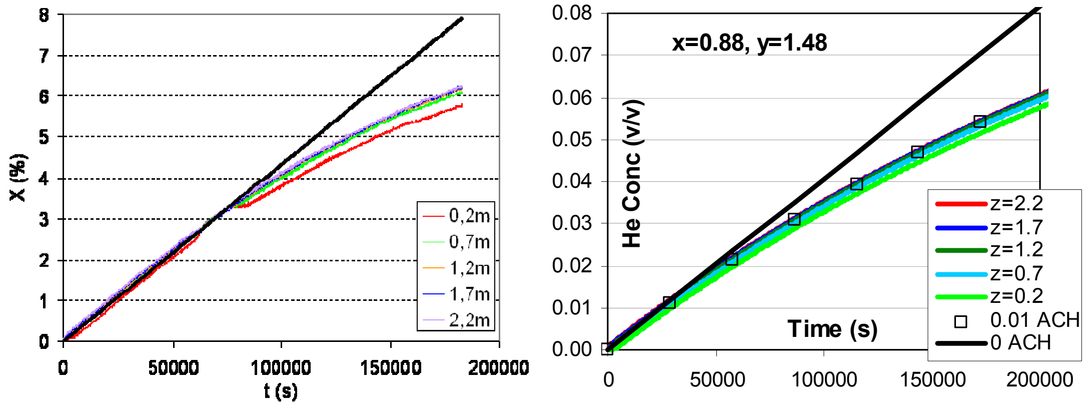
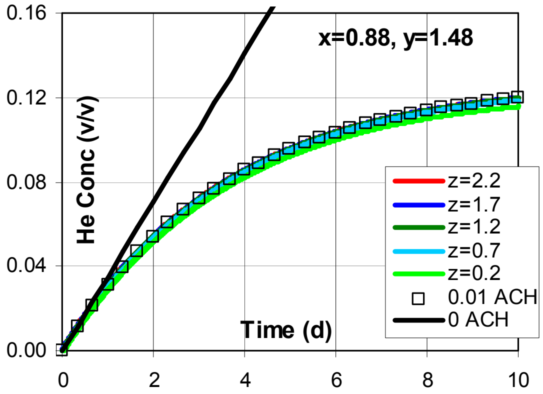


Figure 7 CEA-1: Caption as in Figure 6 but for a release period of 2.3 days.



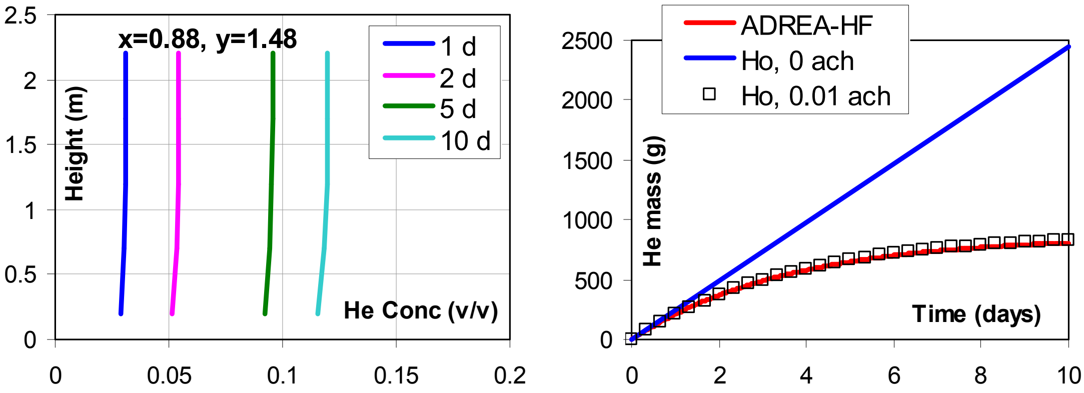


Figure 8 Scenario CEA-1: Caption text as in Figure 4

5.5 Scenario CEA-2

CEA-2 helium dispersion experiments were performed for a release period of 3.5 days. Figure 9 shows a comparison between measured and predicted helium concentration. The CFD simulation is in good agreement with the homogeneous model. A disagreement between CFD and experiments is observed probably because of experimental uncertainty, due to the limiting very low flow conditions used. Both CFD and tests give a 0.02% max concentration difference between ceiling and floor.

Figure 10 (top) shows the predicted concentration time series at various heights from near floor to near ceiling for a release period of 10 days. CFD solution is compared against the homogeneous model. The predicted vertical concentration profiles at various times after start of release are shown in Figure 10 (bottom-left). It is observed that the structure of the concentration profile remains nearly constant with time. Figure 10 (bottom-right) shows the predicted helium mass inside the facility. It is observed that the CFD model accurately predicts the results of the homogeneous model with the same ACH.

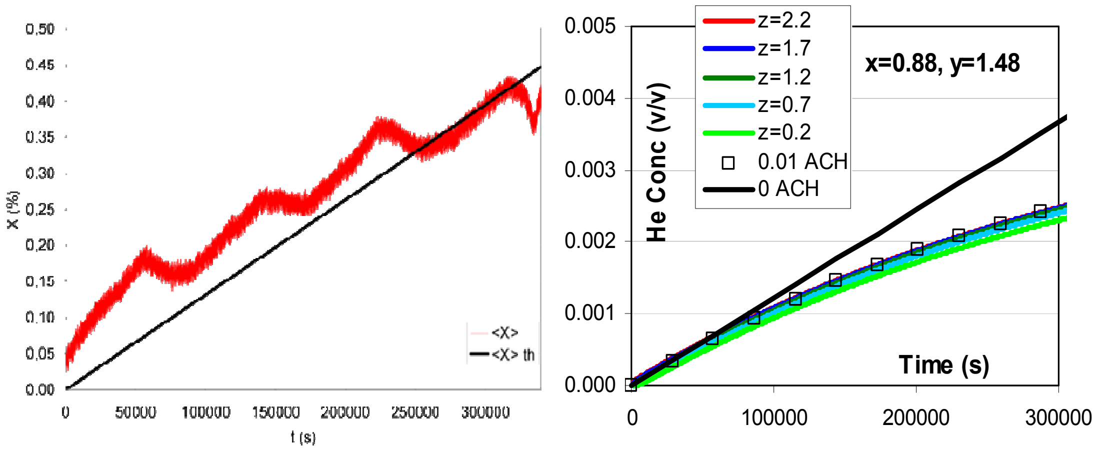


Figure 9 CEA-2: Comparison between measured (left) and predicted (right) concentration time series for a period of approximately 3.5 days. Open boxes and black line show the homogeneous model solution.

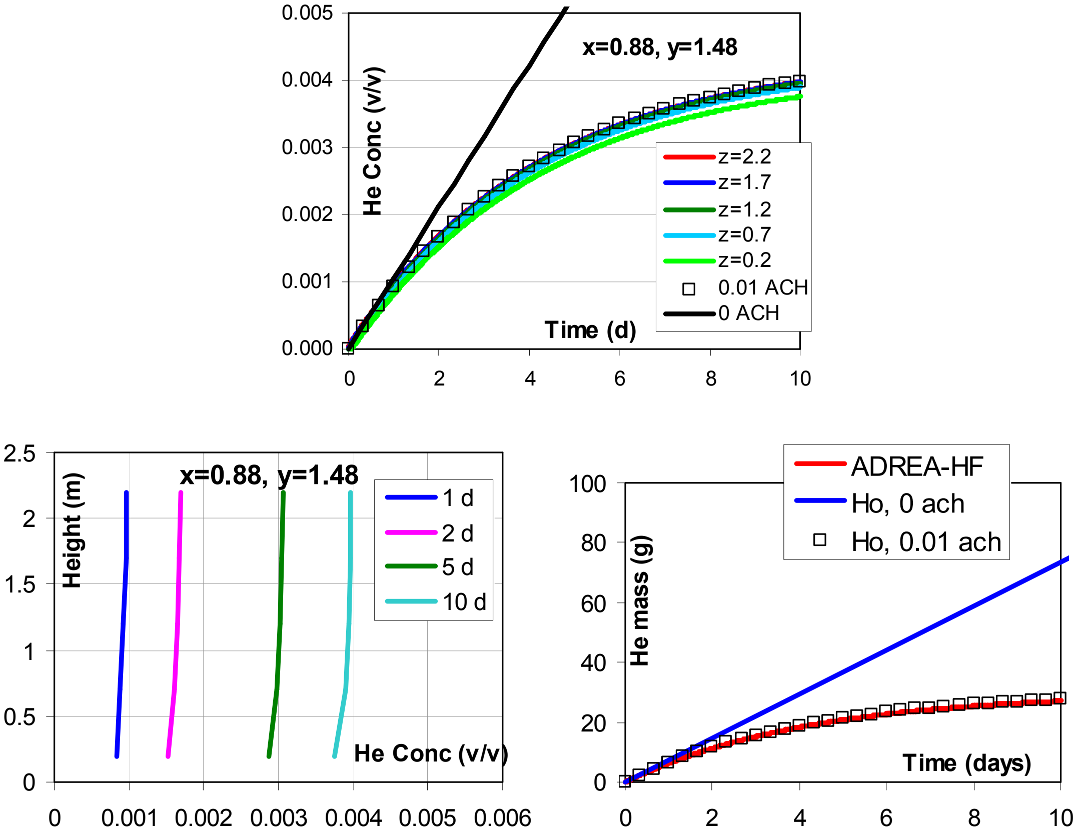


Figure 10 Scenario CEA-2: Caption text as in Figure 4

5.6 Discussion

As mentioned in the abstract the main scope of the present analysis was to check whether permeation releases lead to homogeneous conditions or whether stratified conditions develop.

In view of the results presented above it is necessary to develop a better definition of what is meant by homogeneous or stratified conditions. We define as “homogeneous” the conditions when the concentration difference between bottom and top is much lower than the bottom concentration. If this concentration difference is much higher than the bottom concentration then conditions are considered “stratified”.

With the above definition in mind revisiting the above results shows that scenarios Bus-1, CEA-1 and CEA-2 can be considered as “homogeneous” and scenario Bus-2 as “stratified”. This explains the abovementioned disagreement between CFD and homogeneous model regarding the predicted hydrogen mass in the facility, see Figure 5 (bottom right). The “stratified” conditions in case of Bus-2 scenario can be attributed to the increased level of ventilation rate compared to Bus-1. So increasing ventilation aids “stratification” which leads to higher concentrations, while increasing ventilation lowers the concentrations, due to the higher hydrogen removal rate and the two effects counteract with each other.

Regarding the two-layer model presented in section 3.3 the results presented show that it is not appropriate to be used for permeation releases.

6 CONCLUSIONS

The time and space evolution of the hydrogen distribution in confined settings due to permeation from compressed gaseous hydrogen storage systems was investigated computationally and experimentally. The analysis led to the following conclusions:

- The CFD simulations performed with the ADREA-HF code showed good agreement with the helium dispersion experiments and the homogeneous model. Discrepancy between CFD and measurements for the very low flow rate of 0.03 L/min was attributed to experimental uncertainty due to the very limiting flow rate condition.

- Vertical concentration profiles were observed to be structured as the superposition of the concentration at the floor (driven by laminar diffusion) plus a concentration difference between floor and ceiling (driven by buoyancy forces).

- When the concentration difference is much smaller than the level of the floor concentration, the distribution pattern can be considered as “homogeneous”, while when the difference is much larger than the level of the floor concentration, the distribution pattern can be considered as “stratified”.

- “Stratified” conditions were predicted with the CFD for one scenario. This was attributed to the level of ventilation being large enough. When the ventilation level was very low “homogeneous” conditions were found.

- For the examined scenarios maximum predicted vertical concentration difference between floor and ceiling was 0.5 vol. %.

- For the particular scenario where “stratified” conditions were observed the concentrations predicted by the homogeneous model were within less than 0.5% of those predicted by the CFD.

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