Testing of Novel Application of GOTHIC™ to Modelling of Hydrogen Distribution in Intermediate Level Waste Storage Facilities – 16499

Gustavo Rubio *, Rajan Kumar *, Graham Tucker *
* Atkins Limited, The Hub, 500 Park Avenue, Bristol BS32 4RZ, UK

ABSTRACT

One of the strategies for treatment of intermediate level waste in the United Kingdom is to retrieve the waste from the legacy storage area, condition in a suitable storage container and then hold on-site in an intermediate level waste store until permanent storage in a geological disposal facility becomes available.

During storage, hydrogen may be generated inside the containers at a slow rate by a number of mechanisms. The containers can be equipped with vents that release hydrogen and other gasses into the intermediate level waste store, a building which would be constructed to high standards to minimise ingress of moisture. With the low number of air changes associated with the building design there is the potential for gas to accumulate over time.

There is, therefore, a requirement to be able to predict future gas concentrations inside the building over a range of operating conditions to ensure that a safe operating envelope is maintained.

The usual approach to this problem is to model the evolution of the hydrogen distribution by use of computational fluid dynamics tools. In a situation where weeks of real time need to be simulated in order to understand the slow build-up of a very small volumetric concentration of hydrogen, the use of computational fluid dynamics is not practicable within the time scales demanded by industry. This paper investigates a new approach to tackling this problem using the thermal hydraulic code GOTHIC™[a].

INTRODUCTION

During the operational life of UK nuclear power stations, various forms of ILW were generated and stored on site in a range of facilities including wet or dry underground vaults and above ground tanks. This waste is undergoing retrieval and processing (conditioning) which will enable it to be stored safely until a final repository becomes available.

A number of sites within the UK Nuclear Decommissioning Authority state have adopted the encapsulation strategy whilst others are using a self-shielding container approach.

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[a] GOTHIC™ incorporates technology developed for the electric power industry under the sponsorship of EPRI, the Electric Power Research Institute.

The contents of the containers generate hydrogen due to a range of mechanisms of which the principal one is oxidation of magnesium. Although these mechanisms are well understood, the heterogeneity in the contents of the containers makes it difficult to estimate the hydrogen generation rates.

The hydrogen will be passively vented from the containers and into the store through vents installed on top of the containers. Since the containers are stacked vertically, an exit path is created by the use of spacers fitted to the corner of each container. Gas generated will therefore be able to flow out of the container via the vent, along the narrow path between the upper and lower container, and into the space between the stacked containers. The final hydrogen concentrations in the building will be the result of the combined effect of geometry, molecular diffusion, and the buoyant nature of the hydrogen containing air. Diurnal effects such as the heating of the building by ambient sunlight are also expected to play a role.

The ILW stores are expected to be constructed and operated to a high standard of leak tightness. The effect of this is that the building will have a considerably lower rate of natural air changes than similar industrial structures.

The purpose of this exercise is to understand, in the absence of any active hydrogen control systems, what is the highest volumetric concentration of hydrogen that will occur in the building. Such an analysis can be used to substantiate claims made within the safety cases.

For the situation observed in this paper, lumped parameter codes do not offer the required level of accuracy. On the other hand, the computational time that a Computational Fluid Dynamics (CFD) code would take makes the use of these tools impractical. Using GOTHIC™ allows an improved understanding of the evolution of hydrogen in the building within affordable time scales. The benefits are greater if the variability in the hydrogen generation rates among different containers makes a parametric study necessary.

This paper presents a method to simulate the distribution of hydrogen inside the building using the thermal hydraulics code GOTHIC™. It looks at one deterministic case where all the containers vent hydrogen at a rate of 1 litre per hour.

DESCRIPTION OF THE INTERIM STORAGE FACILITY

The ILW store is essentially a steel framed industrial-grade building. The design considered has a number of significant features to enhance its performance such as providing additional life expectancy and a lower envelope permeability.

The building would be expected to accommodate storage of the specified numbers of containers within a storage area surrounded by a shield wall. For the purpose of this paper, the containers are stored in quadruple height stacks, except the final row that has only two stacked containers. For a building to contain 1,000 containers in this layout, the floor surface area required would be approximately 2,000 m^2.

The building would be designed to maximise its capacity to maintain internal environmental conditions within specified limits by passive means, i.e. without mechanical/electrical intervention. The principal elements of that passive capacity would be its envelope air tightness and its envelope insulation. With reference to the standard building requirements in the UK, where leakage rates are subject to a maximum of 10 $m^3/h/m^2$ at a pressure differential of 50 Pa, for this exercise we have selected a figure of less than 2 $m^3/h/m^2$ at the same differential pressure.

THE GOTHIC™ CODE

GOTHIC™ is a general purpose thermal hydraulics code that is used extensively in the nuclear power industry [1]. It bridges the gap between the lumped parameter codes frequently used for containment analysis (e.g., MAAP, COCOSYS, ASTEC and MELCOR), and CFD codes.

GOTHIC™ solves the mass, energy and momentum equations for three separate phases: vapour, continuous liquid and dispersed liquid (droplets). The vapour phase can be a mixture of steam and non-condensing gases, with a separate mass balance being maintained for each component of the vapour mixture. Within a single model, GOTHIC™ can include regions treated in conventional lumped parameter mode and regions with 3 dimensional flows in complex geometries. This makes it possible to use a variety of noding arrangements in order to accommodate a wide range of modelling needs, while optimizing the use of computational resources. For the solution methods in sub-divided volumes, GOTHIC™ uses a finite volume approach with a first or second order upwind method for the discretisation of convective terms, and a semi-implicit method for time integration.

Although it does not include certain capabilities normally included in CFD codes (e.g., boundary layer analysis), through the use of standard wall functions for heat and momentum transfer, it can give good estimates of the 3 dimensional flows and distributions. This approach reduces the computational time significantly as it allows for the use of coarser spatial meshes while retaining the physical phenomena that are important for modelling hydrogen behaviour. GOTHIC™ has the following capabilities that make it particularly suitable for hydrogen management analysis in containment buildings:

- GOTHIC™ includes the models enabling accurate prediction of gas concentrations: molecular and turbulent diffusion, natural and forced convection, boiling and condensation and multiple component gas mixtures.
- GOTHIC™ allows the use of multiple scales in the same grid.
- GOTHIC™ allows the modelling of complex 3 dimensional geometries with the combination of blockages and openings.

Validation of GOTHIC™

The gas mixing modelling capabilities of GOTHIC™ have been extensively validated in a variety of applications in the civil nuclear industry. A selection of examples of validated applications are presented below.

The Battelle-Frankfurt model containment test facility in Germany [2] was used to experimentally address the issue of the formation of hydrogen during and after a loss of coolant accident in a light water reactor. Test 6 at the facility is a vertical geometry test in combination of three rooms with significant temperature stratification between two rooms. The injected gas was 34% nitrogen and 66% hydrogen by volume. The gas injection rates were such that they resulted in gas velocities on the order of 1 m/hr. The comparison of predicted and measured concentrations shows that GOTHIC™ can accurately predict hydrogen concentrations.

At the Hanford Engineering Development Laboratory (USA) [3], an experimental program was designed to study mixing of hydrogen by natural and forced convection in an air-filled containment. Two tests were selected to assess the ability of GOTHIC™ to accurately predict the transport of non-condensing gases. Test HM-5 simulated a hydrogen-steam release from a horizontal jet into the nitrogen-filled containment for 11 minutes at a rate of 25 kg/min (steam) and 0.3 kg/s (hydrogen). A nitrogen atmosphere was used to avoid the creation of an explosive mixture of oxygen and hydrogen. Experimental results showed that hydrogen is well mixed throughout the test whilst the hydrogen concentrations predicted by GOTHIC™ showed slight discrepancies with the experimental data during the injection phase.

A suite of trials were also performed at the *Heissdampfreaktor* in Germany [4]. The full scale containment experiments begin with a water or steam/water blowdown. Test T31.5 included a secondary injection of steam and injection of a hydrogen/helium mixture into the containment near the point of the steam break, approximately 20 min after the break. The secondary events in test T31.5 are extremely low flow rate events relative to the blowdown. During and after these events, buoyancy is the principal mechanism for mixing. The results of the simulations showed that both GOTHIC™ predictions and experimental data for hydrogen concentration and temperature were consistent.

The *Passive Nachwaermeabfurh und Druckabbau-Testanlage* facility was used as the basis for the assessment of the capabilities of various classes of codes. CFD and lumped parameter codes were used to simulate gas mixing/stratification in large volumes. Analysis of those tests relevant to the distribution of a light gas (helium simulant for hydrogen) are reported in a paper [5] and showed that GOTHIC™ was a viable option to predict gas mixing with a high degree of confidence. In particular, the over-prediction of mixing obtained with lumped-parameter codes and the distortions in the mass transport patterns associated with 1D-system codes could be avoided to a large extent. Building on those previous tests, further experiments were carried out featuring an injection of steam or a mixture of helium and steam in one vessel and gas transport to the adjacent vessel. An overview of the simulations of these experiments with GOTHIC™ using relatively coarse meshes (when compared to CFD meshes) has been reported in a paper [6] and the phenomena were generally correctly represented, giving confidence in the capability of the code to predict gas distribution in a complex geometry.

The code has been shown to be capable of simulating the fast release scenario during a station black out with delayed creep rupture in the hot leg and the prevailing processes governing the mixing of hydrogen with the containment [7]. Heterogeneous local conditions and the formation of a stratified cloud of hydrogen in the dome due to buoyancy-driven flows were well simulated.

Grgić et al [8] calculated the hydrogen concentration at the Krsko nuclear power plant during a design basis loss of coolant accident using GOTHIC™. The model took into account the influence of both original electric and new passive hydrogen recombiners in the build-up and dispersion of hydrogen. The results were used as the basis for sizing of hydrogen recombiners.

GOTHIC™ MODEL DESCRIPTION

In this paper, a slice of an intermediate level waste store with a rectangular cross-section is analysed. The dimensions of the cross-section and the layout of the containers inside it are shown in Figure 1. The containers are stored between shielding walls that are 600 mm thick and 17.8 m apart (outer surface). These shielding walls span along the entire length of the building providing an enclosure. The container stacks are modelled with a horizontal gap of 20 millimetres between each container and the one on top to allow for the hydrogen exiting through the top vents. The stacks of containers are 400 mm apart in the *x* and *y* directions.

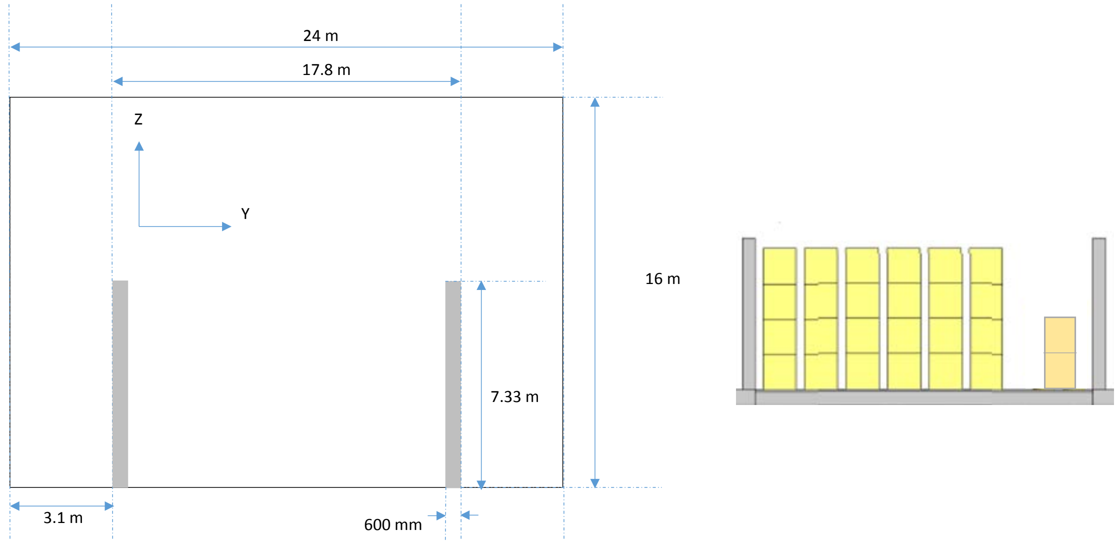

Fig. 1. Building dimensions and containment layout.

The GOTHIC™ model represents a slice of the building with a depth of 12 meters in the *x* direction. Such a slice contains 5 rows of stacked containers. Figure 2 shows a top view of the computational slice (only the area in between the shielding walls).

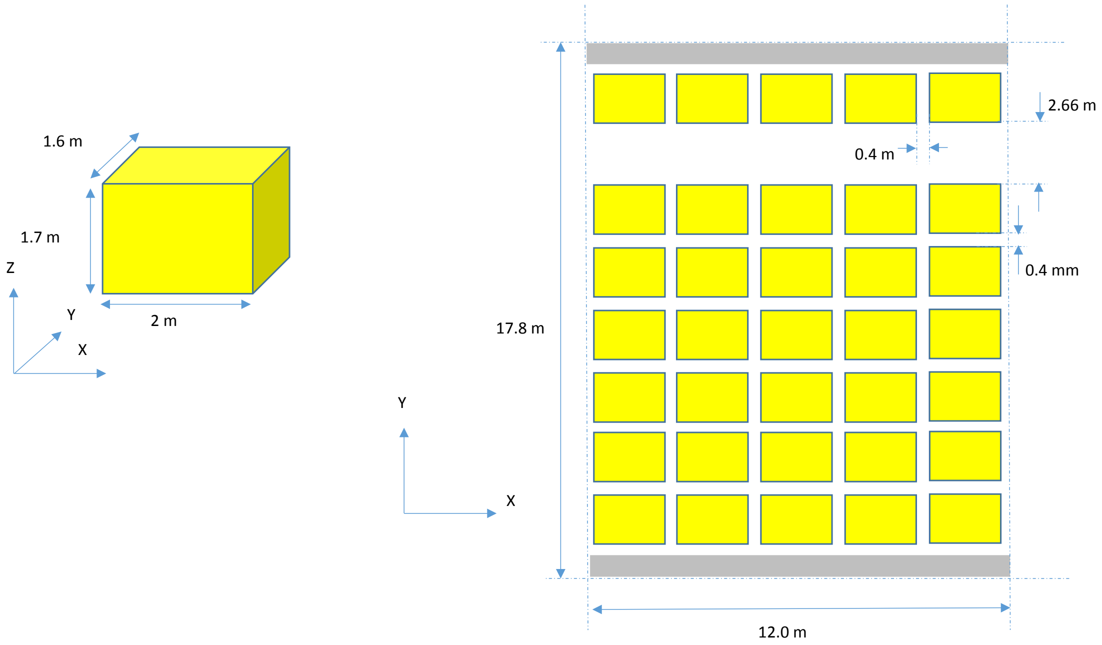

Fig. 2. Containers layout in the computational domain (top view).

The intermediate level waste store has been modelled in GOTHIC™ using two sub-divided volumes as per in Figure 3.

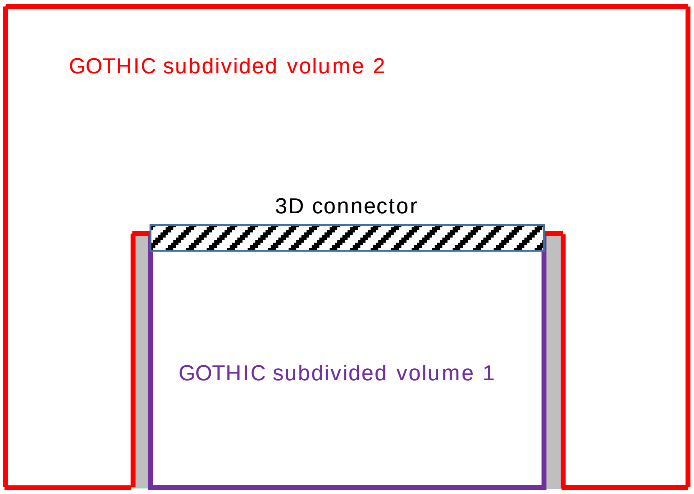

Fig. 3. GOTHIC™ volumes used to model the building.

Volume 1 is the space in between the shielding walls where the containers are located. The volume is subdivided according to the pattern imposed by the containers and the gaps between them both in the horizontal and vertical directions. The cells that are occupied by a container are modelled as a blockage, so that no flow can come in or go out from those cells.

The venting of hydrogen is modelled by applying one individual flow boundary condition on top of each of the containers. The model represents a situation where each individual container is venting 1 litre of hydrogen per hour. Boundary condition parameters are given in Table I.

TABLE I. Hydrogen Venting Boundary Conditions

BC Type	Pressure (kPa)	Temperature (^{0}C)	Flow (l/h)	Air Vol. Fraction	H_2 Vol. Fraction
Flow	101.35	25	1	0	1

Volume 2 is the space above and outside the shielding walls. It has an inverted U shape as can be observed in Figure 3. This shape has been obtained by applying a blockage in the sub-volume that is occupied by volume 1.

The two volumes are connected using a 3D connector that spans the top surface of the space between the shielding walls.

Modelling of the environment and non-specific building leakage

In the absence of any active systems to control hydrogen, air exchange occurring through non-specific leakage is the only mechanism that the building relies on to maintain hydrogen concentration within acceptable limits.

GOTHIC™ includes laminar and turbulent leakage models applicable to both lumped parameter and subdivided volumes. The laminar model is intended to simulate the leakage through narrow cracks where the flow can be characterized as laminar. The modelling option chosen ignores both temperature and pressure effects on the vapour density as it passes through the walls and therefore assumes that the density of the gas stays constant as it passes through the crack. This is deemed to be acceptable as the pressure differential that gives rise to the leakage is of the order of a few Pascals. The viscosity is also assumed to be constant at the reference conditions.

The GOTHIC™ leakage model requires a leakage rate factor (%/hour) at given reference conditions as an input. It has a positive value if the reference pressure is above the pressure in the sink and the leakage is out of the volume. The leakage parameters are given in Table II.

TABLE II. Laminar Leakage Model Parameters

Leakage Rate (%/hour)	Reference Pressure (kPa)	Reference Temperature (^{0}C)	Reference Humidity (%)	Density Option
31	101.4	18	60	Constant

The leakage rate is given for a pressure differential of 50 Pa. The laminar leakage model also requires a leak sink or source which is the GOTHIC™ volume whose calculated conditions include the effects of the leakage. The building leaks into the environment which is modelled using a lumped parameter volume with prescribed boundary conditions. The volume of the environment is 100 times the volume of the portion of the building being modelled in the computational domain. This is chosen to ensure that the leakage will have a negligible influence in the thermodynamic conditions in the environment, so that it will behave according to the prescribed boundary conditions.

The lumped parameter volume simulating the environment has two boundary conditions. These ensure that the simulated environment reproduces the meteorological conditions recorded locally and also that sufficient air exchange is provided, so that the accumulation of energy does not artificially increase the temperature in the environment surrounding the building. It also prevents the build-up of hydrogen in the environment volume. Boundary condition parameters are given in Table III.

The flow boundary condition is defined to generate an inflow of 150 kg/s of air. As the lumped parameter volume simulating the environment contains 460,800 m^3 of air, this means that the air in that volume is changed every hour.

TABLE III. Environmental Boundary Conditions

BC Type	Pressure (kPa)	Temperature (^{0}C)	Humidity (%)	Flow (Kg/s)
Flow	101.35	Recorded[b]	Recorded	150
Pressure	101.35	Recorded	Recorded	N/A

The oscillations in temperature and humidity recorded locally during a characteristic week are shown in Figure 4.

In the model, the pressure of the environment is maintained constant at a value of 101.35 kPa defined at an elevation of 10 m. That is the sink pressure for the leakage model. The 10 meter elevation means that, at the sea level, the pressure is kept constant at a value of, approximately, 101.45 kPa. This represents a worst case scenario (possible over a 150 year potential operational life) where a high pressure weather system is static in the area of the building. The 10 meter difference between the elevation given to the pressure boundary condition in the environment and the

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[b] Temperature and humidity data have been recorded locally at hourly intervals.

elevation of the building in the model does not promote any artificial leakage, as GOTHIC™ uses the elevations to automatically adjust the leak sink pressure, so that the gravitational head is correctly taken into account.

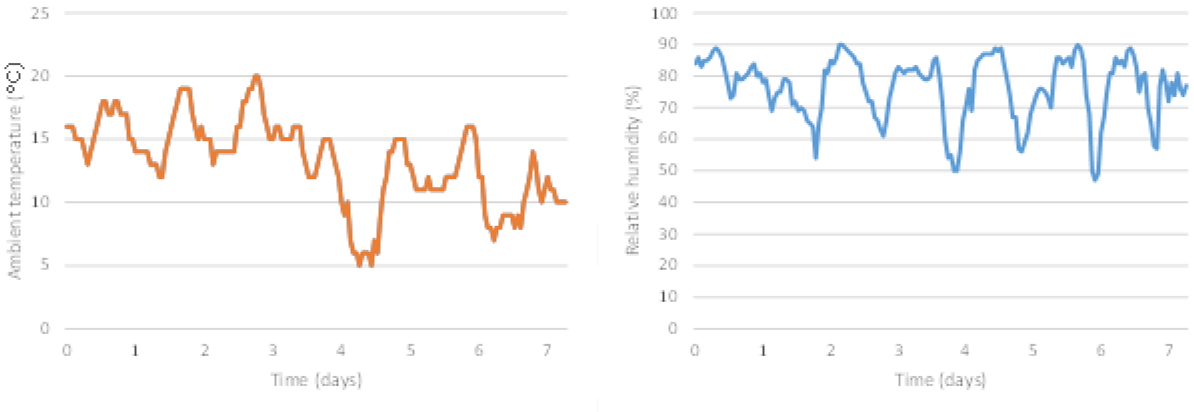

Fig. 4. Ambient temperature and relative humidity oscillations.

Heat gain through the roof

Heat gain through the roof is taken into account by incorporating a spanned thermal conductor in the model. This conductor connects the environment with the atmosphere inside the building through the surface of the roof.

The thermal conductor is modelled accounting for the different construction layers in the roof of the building. These, together with their thermal properties are shown in Table IV.

TABLE IV. Thermal Conductor Modelling Parameters

Material	**Thickness (% of total)**	**Conductivity (W / m / K)**	**Density (kg / m^3)**	**Specific Heat (kJ / kg / ^{0}C)**
Outer skin	0.46	205	2,700	0.91
Air gap	30.54	0.026	1.184	1.005
Insulation	68.73	0.040	10	0.67
Inner skin	0.27	43	7,850	0.49

The surface condition at the inner side of the building is the *direct* option in GOTHIC™. This option applies a condensation and a natural convection model. Since the temperature of the wall stays higher than the saturation temperature inside the building, condensation is effectively set to zero throughout the calculation. For the natural convection model, a correlation is applied based on the Nusselt number as a function of Rayleigh number, with the heat transfer coefficient being determined from this correlation using the fluid conductivity and the cell hydraulic diameter.

For the outside of the building, the surface condition is the *Sp Ambient and HTC* option in GOTHIC™. In this option a nominal ambient temperature is used with a secondary heat transfer coefficient that applies to the heat transfer between the ambient and the surface. The modelling represents the external wall of a building that is exposed to a known ambient temperature connected to the outside surface through a specified heat transfer coefficient model. In order to account for the heat radiation from the sun, the ambient temperature that is used in the model is not the ambient temperature recorded locally, but the sol-air temperature. The sol-air temperature is the temperature of the outdoor air that, in the absence of all radiation changes, gives the same rate of heat entry into the surface as would the combination of incident solar radiation, radiant energy exchange with the sky and other outdoor surroundings, and convective heat exchange with the outdoor air [9]. The convective heat transfer coefficient value is set at 11.35 W/m^2/K.

It is important to note that the current model neglects the heat transfer to the walls and the floor. This is not expected to affect the distribution of hydrogen, but it could have some effect in local volume concentrations, especially in narrow spaces.

CALCULATION OF HYDROGEN CONCENTRATION AND DISTRIBUTION

A single deterministic analysis has been carried out using GOTHIC™. The computation was run for 1,800,000 seconds of real time (3 weeks). This process took 34.5 hours using a four core Xeon 5690 processor @ 3.47 GHz.

Building thermal behaviour

Figure 5 shows the thermal behaviour of the building. The temperature in the simulated environment follows that imposed in the flow boundary condition. The temperature inside the building is, as an average, approximately 5 ^{0}C higher than outside the building. The ambient temperature fluctuations are well reproduced inside the building through the effect of the thermal conductor. The amplitude of these fluctuations is higher in the dome than in other areas of the building and in the gaps between the containers. This can be explained because the effect of leakage in changing the air inside the building is more efficient in the dome.

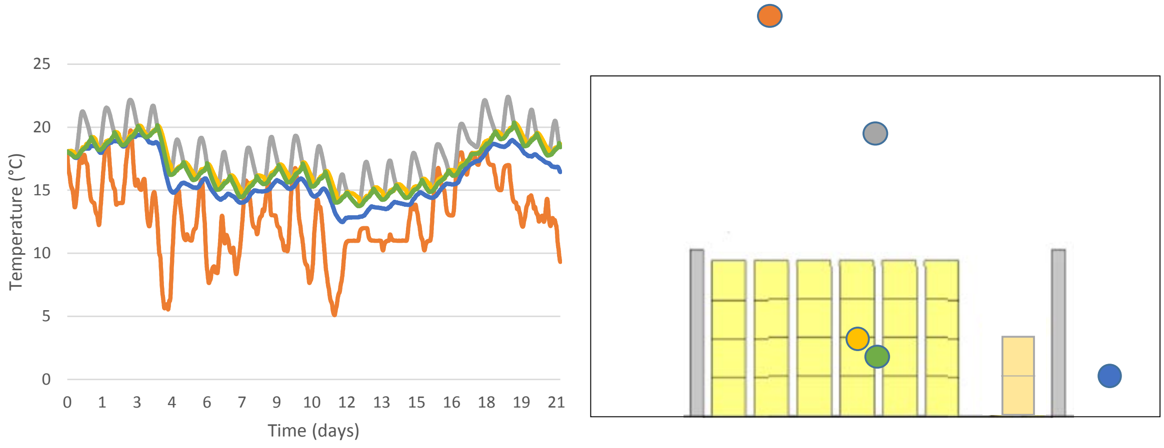

Fig. 5. Building thermal behaviour.

Hydrogen build up and distribution

Figure 6 shows the hydrogen volume fraction at the three gaps of a single container stack and also just above the stack. As expected, the volume concentration of hydrogen is higher between the gaps and oscillates with the temperature fluctuations. The reason for this is that, as the gas constant of hydrogen is much higher than that of air, for a specific temperature change and with the pressure inside the building staying constant, hydrogen expands more than air and occupies more volume.

The gap between the second and third containers shows the highest concentrations, reaching values slightly above 3% after 3 weeks. The concentration above the stack is significantly lower and stays at approximately 1% after 3 weeks.

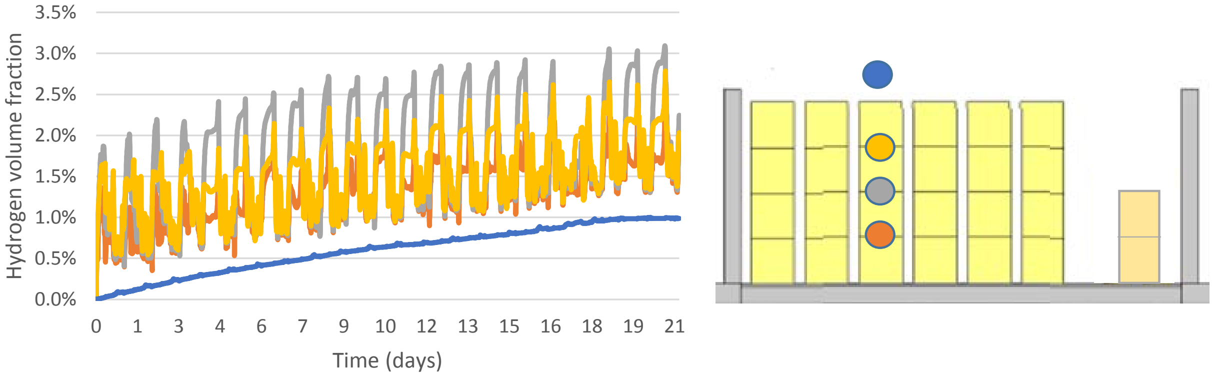

Fig. 6. Hydrogen volume concentrations in between containers.

Figure 7 shows the hydrogen volume concentration at different heights in between 2 stacks. The concentrations are very similar to those found above the stacks. In this case, small peaks of concentration can also be observed coincident with the temperature fluctuations. These peaks also disappear above the stacks.

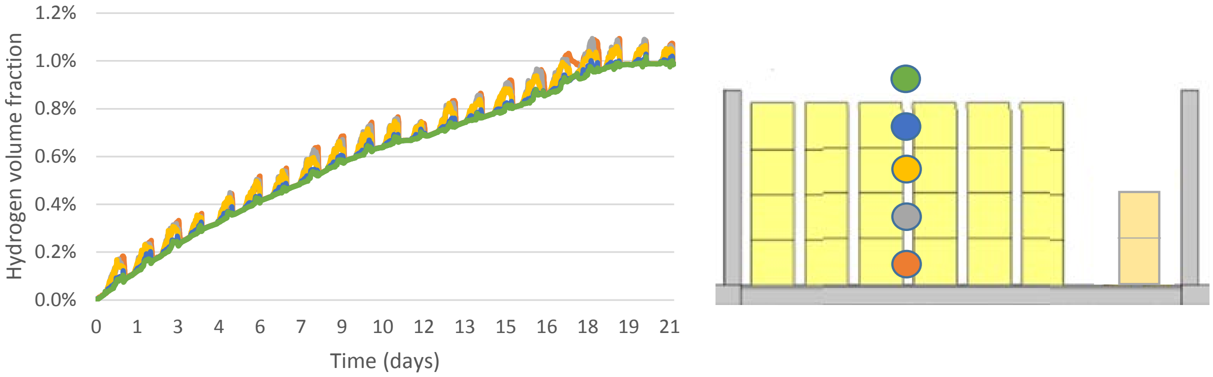

Fig. 7. Hydrogen volume concentrations between stacks.

Outside the area where the containers are stored, in the dome and the space outside the shield walls, the hydrogen volume concentrations are lower. This can be seen in Figure 8, where the concentration is plotted in two locations outside the shield walls and three in the dome. The concentrations in the dome and outside the shield walls evolve in a similar way until up to approximately 3.5 days. After that, the concentrations in the dome grow faster until they appear to reach a plateau after 18 days. During the same period, the concentrations outside the shield walls grow with a smaller slope and they start a decrease after approximately 17.5 days. Small fluctuations are observed in the concentrations outside the shield walls, whereas the concentrations at the dome grow more steadily.

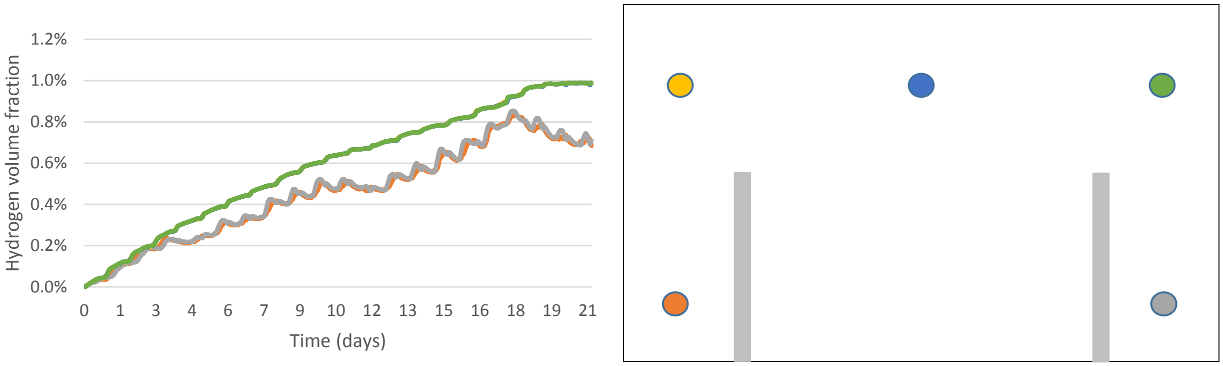

Fig. 8. Hydrogen volume concentrations in open spaces.

Figure 9 shows the evolution of the total mass of hydrogen accumulated in the building. The amount of hydrogen grows quasi-steadily at a rate of 7.2 grams per hour (average) from the beginning until approximately 18 days. At the end of the calculation the building has accumulated 3.1 kg of hydrogen.

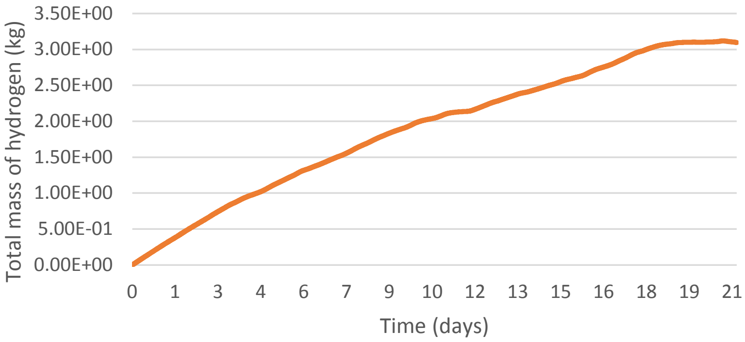

Fig. 9. Evolution of the total mass of hydrogen in the building.

The model has 130 boundary conditions (one per container). Each of them injects hydrogen at 101.35 kPa and 25 ^{0}C at a rate of 1 litre per hour or, under those conditions, 2.361×10^{-8} kilograms per second. After 3 weeks, and if no hydrogen had left the building through leakage, the total amount of hydrogen in the building should be 5.57 kg. By mass balance, 2.47 kilograms of hydrogen have been lost through leakage.

The leakage rate is shown in Figure 10.

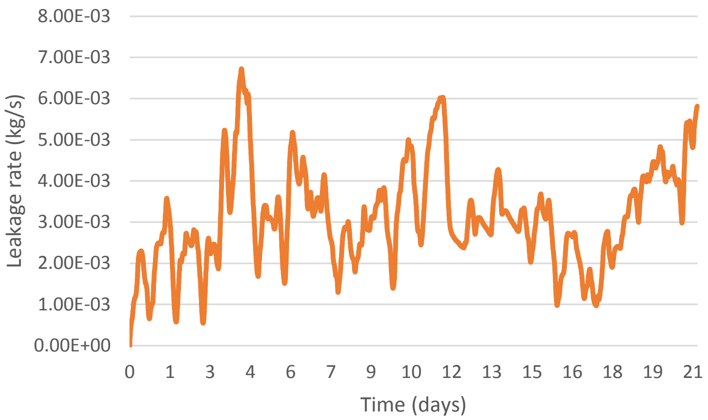

Fig. 10. Leakage rate.

Integrating the curve in Figure 10 shows that over the three weeks, 5,618 kg of gas mixture (air and hydrogen) have left the building through leakage. As an average, the volume fraction of hydrogen in the gas mixture leaking from the building is 0.59% which seems reasonable.

CONCLUSIONS

Thermal hydraulics code GOTHIC™ has been used to model the build-up and distribution of hydrogen inside an intermediate level waste store. The model includes non-specific leakage of the building, heat transfer into the building from solar radiation and the real environmental conditions that the building would be exposed to. A deterministic worst case scenario has been selected where the pressure stays constant at a value slightly above standard atmospheric at the sea level, for a period of 3 weeks. The model contains 130 containers each of them venting hydrogen at a rate of 1 litre per hour.

The model reproduces the thermal behaviour of the building during the day and night cycles, and is able to capture the slow build-up of small concentrations of hydrogen in the building. The results display differences in hydrogen volume concentrations between the small spaces in between the containers and the open spaces in the dome and outside the shielding walls.

Small pressure oscillations inside the building drive the leakage of a mixture of hydrogen and air from the building. Hand calculations show that the mass of hydrogen accumulated in the building at the end of the computation is consistent with a leaked average hydrogen mass fraction of 0.59%.

At the end of the 3 weeks, the volume fraction of hydrogen in the building is stable and around 1% or less in the open spaces (dome and outside shielding walls). In the space in between container stacks, the volume fraction of hydrogen is similar to that in the open spaces. In the spaces in between containers, the volume fractions of hydrogen oscillate with the day and night temperature cycles. Those oscillations reach peaks of 3.1% after 3 weeks.

Even if the concentrations outside the shielding walls at the lower levels of the building are lower than those observed at the dome at the end of the analysis, no significant stratification is observed in the analysis.

A number of features can still be included to increase the accuracy of the results. Notably, the heat losses through the building floor are likely to change the relative temperature difference between the atmosphere inside and outside the building. This might have an effect in the amplitude of the local temperature oscillations inside the building and, ultimately, in the maximum hydrogen volume concentrations that will be observed in the area where the containers are stored.

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