Hy4Heat
demonstrating hydrogen for heat

Department for Business, Energy & Industrial Strategy

WORK PACKAGE 7

Safety Assessment:

Gas Dispersion Modelling Assessment

WP7 SAFETY ASSESSMENT

The Hy4Heat Safety Assessment has focused on assessing the safe use of hydrogen gas in certain types of domestic properties and buildings. The evidence collected is presented in the reports listed below, all of which have been reviewed by the HSE.

The summary reports (the Precis and the Safety Assessment Conclusions Report) bring together all the findings of the work and should be looked to for context by all readers. The technical reports should be read in conjunction with the summary reports. While the summary reports are made as accessible as possible for general readers, the technical reports may be most accessible for readers with a degree of technical subject matter understanding.

Safety Assessment:
Precis
An overview of the Safety Assessment work undertaken as part of the Hy4Heat programme.

Safety Assessment:
Conclusions Report
(incorporating Quantitative Risk Assessment)

A comparative risk assessment of natural gas versus hydrogen gas, including a quantitative risk assessment; and identification of control measures to reduce risk and manage hydrogen gas safety for a community demonstration.

Safety Assessment:
Consequence Modelling Assessment
A comparative modelling assessment of the consequences in the event of a gas leak and ignition event for natural gas and hydrogen gas.

Safety Assessment:
Gas Ignition and Explosion Data Analysis
A review of experimental data focusing on natural gas and hydrogen gas ignition behaviour and a comparison of observed methane and hydrogen deflagrations.

Safety Assessment:
Gas Dispersion Modelling Assessment
A modelling assessment of how natural gas and hydrogen gas disperses and accumulates within an enclosure (e.g. in the event of a gas leak in a building).

Safety Assessment:
Gas Dispersion Data Analysis
A review of experimental data focusing on how natural gas and hydrogen gas disperses and accumulates within an enclosure (e.g. in the event of a gas leak in a building).

Safety Assessment:
Gas Escape Frequency and Magnitude Assessment
An assessment of the different causes of existing natural gas leaks and the frequency of such events; and a review of the relevance of this to a hydrogen gas network.

Safety Assessment:
Experimental Testing - Domestic Pipework Leakage
Comparison of leak rates for hydrogen and methane gas from various domestic gas joints and fittings seen in typical domestic gas installations

WP7 SAFETY ASSESSMENT

Safety Assessment:

Experimental Testing – Commercial Pipework Leakage

Comparison of hydrogen and methane leak rates on a commercial gas pipework system, specifically the gas meter and equipment contained within the Plant Room of a MOD site.

Safety Assessment:

Experimental Testing - Cupboard Level Leakage and Accumulation

Comparison of the movement and accumulation of leaked hydrogen vs. methane gas within cupboard spaces in a typical domestic property.

Safety Assessment:

Experimental Testing - Property Level Leakage and Accumulation

Comparison of the movement and accumulation of leaked hydrogen vs. methane gas within a typical domestic property.

Safety Assessment:

Experimental Testing - Ignition Potential

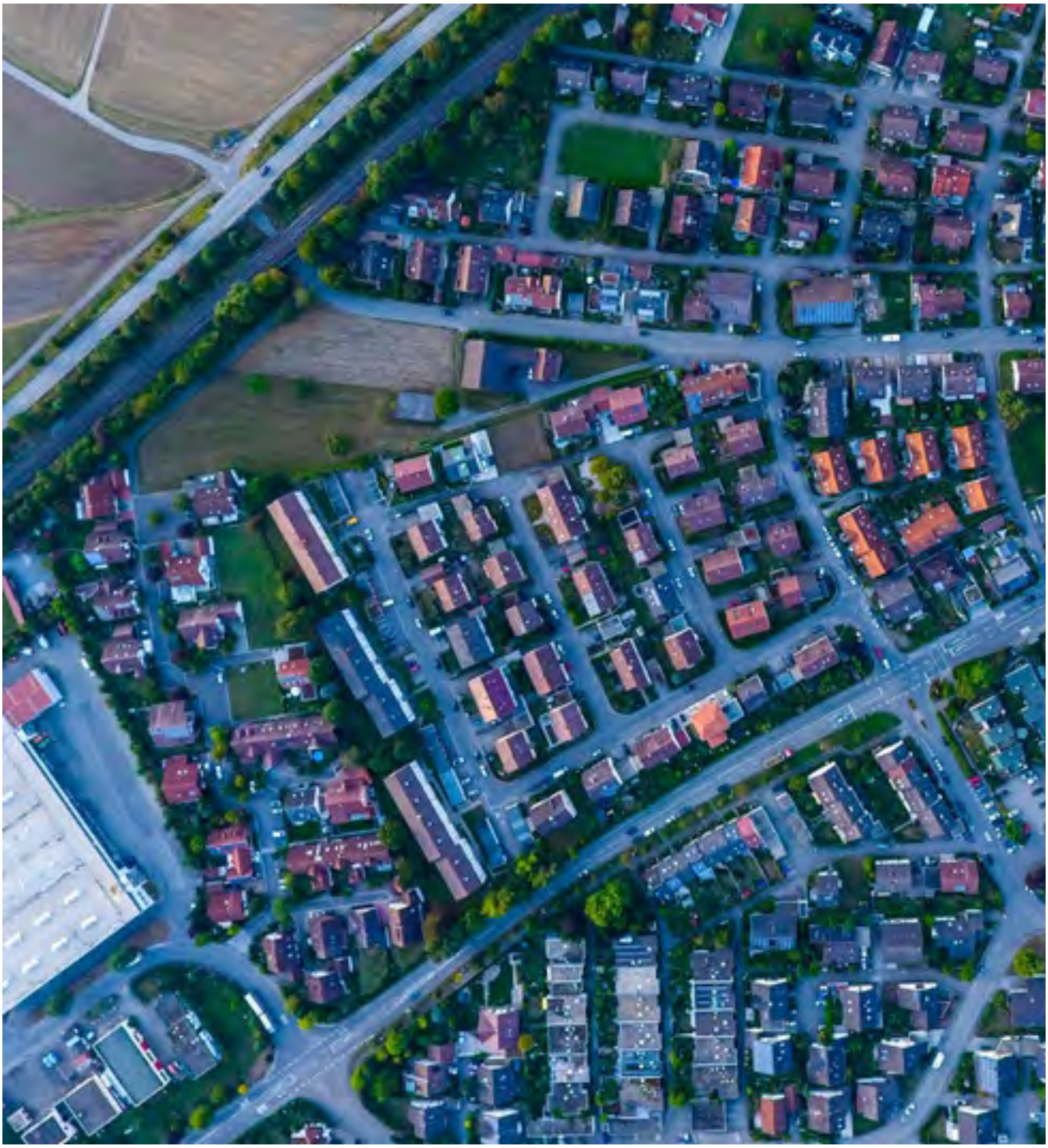
Investigation of the ignition potential of hydrogen-air mixtures by household electrical items and a comparison with the ignition potential of methane-air mixtures.

ARUP

Hy4Heat

Gas Dispersion Modelling Report

1.0 | 1 May 2021



ARUP

Department for Business, Energy & Industrial Strategy

Hy4Heat

Gas Dispersion Modelling Report

ARP-WP7-GEN-REP-0002

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Contents

Tables

Figures

Executive Summary

The assessment of safety risks of hydrogen usage in domestic environment requires methods to characterise the release of hydrogen and natural gas and the gas concentration build-up inside enclosed areas, which are very important parameters in the establishment of the associated consequences in an event of an ignition leading to an explosion.

This report summarises the work undertaken within the Hy4Heat Work Package 7 (WP7), part of the Hy4Heat project for the dispersion modelling of hydrogen releases in a domestic environment.

In this study, fundamental features of hydrogen dispersion for different cases in simple geometries that can be used in the Quantitate Risk Assessment (QRA) framework are presented in order to assess potential and practical hydrogen release scenarios within a domestic environment. Simplified mathematical dispersion models (i.e. Linden model and Molkov model) have been identified and investigated to predict the dispersion of hydrogen and natural gas releases within an enclosure. Validation studies have been provided along with the presentation of the key assumptions considered in the dispersion modelling.

Through benchmarking with available published data and the experimental work undertaken within the Hy4Heat Work Package 7 (WP7), it is demonstrated that the selected dispersion models are reliable, effective and relatively inexpensive tools to evaluate the effects of gas releases in a domestic environment. Conclusions emphasized include:

- Overall, the selected analytical models provided reasonable predictions of most experiments.
- Simplified methods can be used to estimate the concentration reached in an enclosure in case of accidental leak, provided that the main assumptions of the models are valid:
  - The leak is at a level close to the floor: For height of release close to ceiling, reduced agreement is observed between the theoretical results and experiments.
  - The leak rate is low, i.e. the leak hole diameter < ~ 10mm
- Where the simplified models underestimate the dispersion characteristics, the consequence model is developed to consider stratification of hydrogen (and methane) using the estimated height of the peak concentration layer obtained from the simplified models (i.e. two-vent model) and the observations of the WP7 experimental results.
- Based on the observations from the WP7 experimental data hydrogen and methane concentration charts have been developed to be included in the QRA framework to represent spaces within a typical domestic house considering the dimensions of the spaces used for WP7 test programme.

1. Introduction

The Hy4Heat Work Package 7 (WP7), part of the Hy4Heat project, has produced a quantitative risk assessment (QRA) that assesses hydrogen as a potential replacement for natural gas in the domestic environment. The QRA compares the accidental dispersion and consequences of a dispersion event for both natural gas (here assumed to be methane, CH4) and hydrogen (H2) in the domestic environment.

This report summarises the work undertaken within WP7 of the Hy4Heat project aiming to:

- Identify accurate, simple, rapid and validated dispersion models for hydrogen (H2) and methane (CH4) build-up in enclosed areas
- Validate available dispersion models against numerous experimental data
- Identify the limitations of the models based on the comparison study
- Integrate the dispersion model to the hydrogen and methane-specific quantitative risk assessment (QRA), where H2 and CH4 concentration data is provided to the consequence assessment for a given leak scenario as defined in
- Integrate dispersion model output, i.e. concentration data for H2 and CH4 into the QRA so that the potential consequences of a dispersion in a domestic environment can be assessed for hydrogen and compared to the consequences for natural gas, i.e. methane.

Throughout the report, validation and use of identified dispersion models are provided along with the presentation of the key assumptions considered in the dispersion modelling. These models are then used to provide concentration of hydrogen or methane in the domestic environment for the QRA with a better knowledge of their capabilities and limitations.

1.1 Gas dispersion

The leakage mechanism of hydrogen or methane into the air is a significant part of the QRA. Dispersion is a process where the gas will mix with the surrounding air, creating a mixture which might lead to a flammable atmosphere. For instance, when methane or hydrogen leakage occur, the gas tends to react with oxygen which would form a cloud and part of it could be flammable. Dispersion characteristics of hydrogen and methane differ as the physical properties of methane and hydrogen are different: Hydrogen is a low-density gas with wide flammable limits (4%-75% volume), however its stoichiometric mixture is circa 29% volume per volume (v/v) in air, compared with 10% v/v for methane, requiring about three times the concentration of hydrogen in the air when compared to gas. While the behaviour of methane is relatively well understood in comparison to hydrogen, as part of safety studies comparing the use of hydrogen and methane in confined spaces, it is important to have a good understanding of the dispersion and stratification of a hydrogen leak in order to better determine the possibility of ignition and explosion of accidental releases which might lead to the following hazards:

- Formation of flammable mixture that could potentially combust if ignited
- Structural damage of the enclosure or building due to pressure peaking phenomena
- Displacement of breathable air that can result in asphyxiation.

There have been several studies aimed to understand the dispersion of hydrogen in an enclosed space, experimentally and numerically through simplified models or the use of computational fluid dynamic

(CFD) codes. In addition, many research projects, such as HySafe [3], HyIndoor [4], H21 [5], HyHouse [6] have been conducted. All these studies and projects are reviewed within the scope of this work to bring capabilities and experiences from various research regarding hydrogen safety issues. Additionally, newly conducted experimental data within Hy4Heat WP7 is assessed and the observations are summarised in Hy4Heat WP7 Gas Dispersion Assessment report, KIW-WP7-HSE-REP-0002 [7].

2. Concept of dispersion in an enclosure

Several parameters can affect the dispersion behaviour of a gas when released in an enclosure:

1. Release conditions (gas density, flow rate, pressure, exit velocity, exit temperature, location, duration, direction)
2. Enclosure geometry (size and shape of enclosure, size, shape and location of ventilation openings, congestion)
3. Atmospheric conditions both inside and outside the enclosure (ambient temperature, mechanical ventilation, presence of wind)

Gaseous releases through a hole are produced as a result of a positive pressure difference between a pipe/container and its environment. Depending on the pipe pressure, the flow through a hole to a lower pressure can either be choked (or sonic) or subsonic. For hydrogen, a sonic or chocked release would occur when the upstream pressure is 1.9 times larger than downstream, otherwise the flow is subsonic [8]. Similarly, for methane this ratio is 1.84 [8]. For in-house distribution systems, where the average pressure is 20 mbar, the release can be characterised as subsonic.

Methane, with a density of 0.68 kg/m^3 at 15°C and atmospheric pressure, is lighter than air (1.225 kg/m^3), while hydrogen is 7.5 times lighter than methane (0.09 kg/m^3). For the same leak size and pressure, the volumetric flow of hydrogen will be higher than methane, approximately 1.2 times for laminar flows rising to 2.8 times for turbulent flows [9].

Figure 1 below summarises the behaviour of unignited gas releases for varying source pressures. The flow from a subsonic release takes the form of an expanded jet. The concentration profile of hydrogen or methane in this expanded jet is inversely proportional to the distance to the nozzle along the axis of the jet. At a given distance from the nozzle, the concentration profile in air is distributed according to a Gaussian function centred on the axis.

The jet, while momentum-driven at first, becomes buoyancy-driven as a light gas cloud, rich in hydrogen or methane is developed near the leak, which is less dense than air in the room (Figure 1).

In summary, six stages of a hydrogen release in a confined environment can be identified ([8], [10]):

4. Leakage: A hydrogen plume is formed that rises up to the ceiling from where it tends to expand and disperse. The concentration in the plume depends mainly on the leak flow rate and the distance from the leaking point to the ceiling. In this phase, the hydrogen is concentrated mainly on the ceiling and in the plume, whose position depends on the leaking point. During this period, the hydrogen transport is momentum- and/or buoyancy-driven.
5. Jet: The flow resulting from a subsonic release is an expanded jet, where the concentration profile of gas is inertia driven and inversely proportional to the distance to the leak location.
6. Buoyant plume: Buoyant gas is lighter than air and becomes a buoyant cloud, forming a buoyant plume near to the leak. The density difference induces a vertical buoyant force, making buoyant gas rising up with the heavier atmosphere air dropping down in the enclosed space.
7. Stratified dispersion: The buoyant plume mixes with the surrounding air in a non-homogeneous way. When the plume reaches the top of the enclosure, it spreads to the ceiling and stratified conditions

could occur, especially where there is no ventilation mechanism. The concentration of the stratified gas depends on the release location and the geometrical aspect ratio (slenderness) of the enclosed space.

8. Homogenisation: In the medium and long-term, the concentration of hydrogen in each point could move towards homogeneous conditions due to mixing phenomena.
9. Convective and venting phenomena: Final distribution of the buoyant gas depends on the heat transfer (mainly by convection), venting systems, connection to other rooms, fan coolers, etc. Also, any mitigation systems included in the enclosed environment can change the stages of hydrogen release.

All these phenomena yield the final distribution of the gas within the confined environment: well-mixed, stratified, locally accumulated, etc.

Local accumulation usually happens in regions with dead-end enclosures, badly ventilated which obstruct the dispersive motions of the gas. Stratification usually happens close to ceilings and consists on forming stable layers in which gas is in motion but mixing between layers does not occur.

Mixing patterns within the enclosure are induced by jets, plumes and convective heat transfer, which induce moments in the fluid, producing the competition between inertia and buoyancy. When the inertia forces are dominant, the enclosure atmosphere will get mixed, while when buoyancy prevails, the stratification remains.

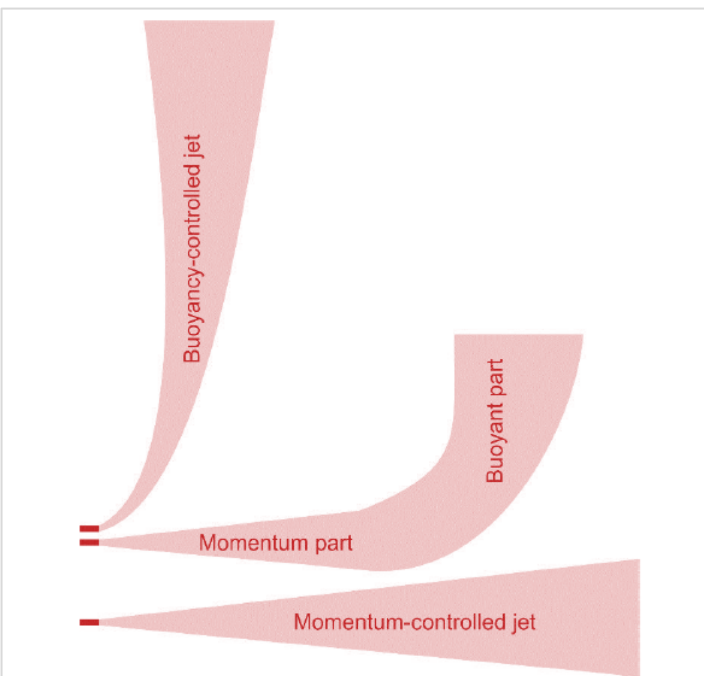

Figure 1: Behaviour of unignited gas releases for varying source pressures

3. Gas dispersion modelling

The purpose of dispersion modelling of gaseous releases is the calculation of the concentration and distribution of gas in a confined environment. The study of hydrogen dispersion in enclosed spaces is especially important from the point of view of safety because useful information can be gained to support the consequence model of the developed QRA framework [11] and define the optimal ventilation strategies.

A wide range of models of different complexity exist to predict the dispersion phenomena after accidental releases, varying in quality and applicability, ranging from simple box models through to more complex three-dimensional computational fluid dynamics (CFD) models. Although the majority of the recent studies on hydrogen safety (e.g. HyIndoor [4], H21 [5], etc.) enclosed environments lean towards using CFD to model gas releases and dispersion to inform their QRA process, this work focuses on phenomenological models in order to simplify and facilitate a faster and repeatable but informed QRA process. There are an almost infinite number of variables in a real domestic environment and so simulating the great variety of potential effects and knowing which to prioritise is an immensely difficult task. Further, whether or not a large and complex CFD simulation produces accurate results depend on the degree of uncertainty and on the cumulative effect of various errors, so it would need experimental work to verify it in any case. Therefore, a literature review of the simple analytical approaches developed for the prediction of the dispersion and final concentration of hydrogen in a room or enclosure was undertaken.

For a given release of hydrogen or methane, the dispersion modelling takes into account the following variable:

- Initiating events that can result in gas release
- Critical factors that may affect the dispersion, such as the sealing conditions of the confined space

Details of these factors are presented in the subsequent sections.

3.1 Initiating events – gas leaks

The Hy4Heat programme focuses on hazardous scenarios arising inside a residential house. Hence, the initiating events for gas leaks occurring within a residential house and their likelihood are first established within the event tree, which is included in the QRA report [12]. An interface with external gas leaks seeping inside the property is also considered as an initiating event for the potentially hazardous scenario occurring inside the property.

3.1.1 Leak hole sizes

A range of leak sizes corresponding to accidental leaks observed in domestic environments have been considered. These include loose or damaged fittings and holes in pipework and have been translated to equivalent hole sizes. The hole sizes start from 3mm up to 15mm. Whilst it is possible to envisage larger holes occurring within domestic pipework, for instance from a full-bore rupture of internal pipework, the selected maximum leak size is assumed to be representative of the maximum that can be sustained by the system into a property. Details of the assumed leak hole sizes are included in Arup's WP7 QRA report [12] and Kiwa's WP7 Gas escape, frequency and magnitude assessment report [13] .

3.1.2 Leak flow rate

The calculation of the volumetric flow rate from a leak source is done using formula B.3 for subsonic releases, proposed by the British Standards Institution, Annex B, BS EN 60079-10-1:2015, Eqn. B.3 [14]:

$$W_g = C_d S p \sqrt{\frac{M}{ZRT}\frac{2\gamma}{\gamma-1}\left[1-\left(\frac{p_a}{p}\right)^{(\gamma-1)/\gamma}\right]}\left(\frac{p_a}{p}\right)^{1/\gamma}\ (kg/s) \qquad (1)$$

where,

W_g	mass release rate of gas (kg/s)
C_d	discharge coefficient (dimensionless) which is a characteristic of the release openings and accounts for the effects of turbulence and viscosity
S	cross section of the opening (hole), through which the fluid is released (m2);
p	pressure inside the container (Pa);
p_a	atmospheric pressure (Pa);
M	molar mass of gas or vapour (kg/kmol);
Z	compressibility factor (dimensionless);
R	universal gas constant (8314 J/kmol K);
T	absolute temperature of the fluid, gas or liquid (K);
γ	polytropic index of adiabatic expansion or ratio of specific heats (dimensionless);

3.1.3 Gas release locations

Most simple models found in the literature assume a leak at floor level approximately in the centre of the enclosure, however experiments have shown that the location and direction of leak is also a contributing parameter to the dispersion behaviour [3]. Accordingly, Table 1 below summarises the spaces that are considered in this work to represent spaces within a typical house considering the dimensions of the spaces used for the Lot 2 and Lot 3 programme of experiments within Work Package 7 (WP7) of the Hy4Heat project ([15], [16]):

Table 1: Gas leak locations and assumed areas

Gas leak locations	**Small confined space (e.g. cupboard)**	**Medium space (e.g. kitchen)**	**Large space (e.g. downstairs of a terraced house)**
Space dimensions (width x length x height)	1.2m x 0.6m x 1.2m	4m x 3m x 2.4m	8m x 4m x 2.4m
Volume size (in approximation with potential leak locations)	~1 m^3	~ 30 m^3	~75 m^3

3.2 The effect of enclosure ventilation and airtightness on gas concentrations

The use of hydrogen or natural gas in a domestic environment is accompanied by a level of ventilation, hence models accounting for this parameter are investigated. The vent configuration has a significant effect on gas accumulation within an enclosure, meaning that each model applies to a specific vent configuration assumption.

Wind is another critical factor influencing the gas accumulation in an enclosure. The effect of wind is difficult to capture using simple models and is not considered in this study.

Only natural forms of ventilation within the compartment areas are accounted for. It is assumed that all external windows and doors are closed. Although models have been proposed for wind-driven ventilation, ignoring buoyancy [3] [17], and wind may be helpful in preventing gas accumulation for certain directions and speeds, it can also prevent the hydrogen from exiting the enclosure through the vents. Also, it is noted in previous studies that the proposed analytical models used in this project remain conservative in most of the cases regarding the calculated concentrations inside semi-confined enclosures [18]. Therefore, no accountability will be made for wind direction and speed.

3.2.1 Vents

The location and sizes of vents affect the dispersion characteristics displayed in the room. The location and quantity of vents influence the gas release mixing behaviour. Such that the mixing within the space can result in homogenous mixing or gas stratification.

3.2.2 Air leakage

In addition to vent areas such as vent ducts, windows, or doors, there are additional air leakage paths in a dwelling including:

- Cracks, gaps and joints in the structure
- Pathways through floor, ceiling voids into cavity walls and then to the outside
- Leaky windows or doors
- Service penetrations through ceilings
- Vents penetrating the ceiling, roof, walls
- Gaps around kitchen pipes
- Gaps in and around electrical fittings in walls
- Open chimneys

Whilst values of airtightness characteristics of residential buildings can be found in the literature such as the guidelines for commercial and public Buildings [19], Building Regulations ([20], [21]) and the assessment of Lot 2 and Lot 3 data within Work Package 7 (WP7) of the Hy4Heat project ([15], [16]), there is some uncertainty as to how air tightness could be translated to vent area in a room instead of whole building for a specific volume.

Based on the review of the above-mentioned references, three different level of airtightness are considered for the development of dispersion models:

- Highly sealed
- Moderately sealed
- Leaky

For comparison purposes between different dispersion models, three arbitrary air tightness values, i.e. 3 $m^3/(hr/m^2)$, 5 $m^3/(hr/m^2)$, and 10 $m^3/(hr/m^2)$ are selected, representing typical sealed, moderate and leaky dwelling scenarios, respectively. For development of the dispersion charts to be used in the QRA framework, measured concentrations from the gas dispersion and accumulation data collected by DNV GL within Work Package 7 (WP7) are used to define equivalent vent areas for each enclosed space (i.e. cupboard, kitchen, and downstairs of a terraced house) based on the test vent settings (e.g. doors closed or left open, introduction of vent holes). These equivalent vent areas then used to predict the air permeability rate which is typically used to measure the airtightness of the airtightness of the building fabric. “Air permeability rate” is defined as air leakage rate per hour per square meter of envelope area at a reference pressure differential across the building envelope of, typically, 50 Pascal (50 N/m^2).

4. Description of dispersion models

The following analytical models are studied in Hy4Heat to calculate hydrogen and methane gas build-up in an enclosure considering the air-permeability rate and natural ventilation of the domestic setting:

- Models with one-vent configuration:
  - The model with natural ventilation proposed by Linden et al. [22] with the simple expression developed by Cariteau and Tkatschenko [23] is validated and usable. This model is referred as 'Linden model' in this report.
  - The model with passive ventilation proposed by Molkov et al. [24], which is referred as 'Molkov model' in this report.
- Models with two-vent configuration:
  - The natural ventilation approach proposed by Linden [22]

The details of the dispersion models are described below:

Linden et al. [22] investigated the behaviour of a buoyant jet in an enclosure equipped with **one or two vents**, identified two regimes and proposed a simple analytic model for the calculation of the **steady-state concentration** of hydrogen for each;

i. One-vent mixing (Figure 2): A **well-mixed** regime for the single opening case where

$$\bar{x}_h = \left(\frac{Q_o}{C_D A (g' H)^{1/2}}\right)^{2/3} \quad (2)$$

where, Q_0 is the release rate (m3/s), C_D is vent discharge coefficient (0.60 is recommended), A is vent area (m2), H is vent height (m), g' is reduced gravity $g' = g(\rho_{air} - \rho_{h_2})/\rho_{air}$ (m/s2), ρ_{air} and ρ_{h_2} are density of the air and hydrogen, respectively, (kg/m3).

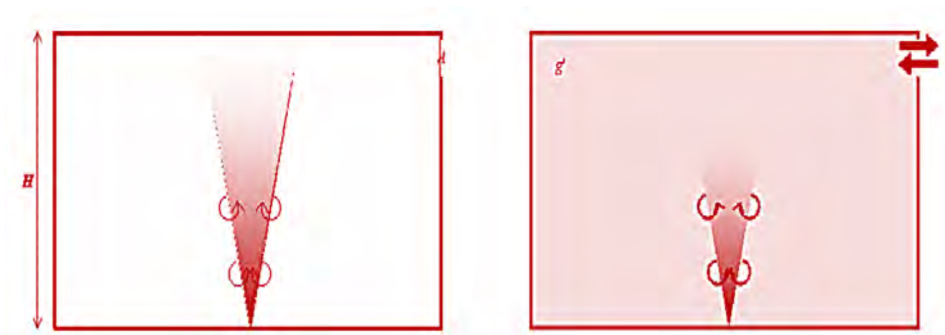

Figure 2: Idealised one-vent mixing ventilation scenario leading to well-mixed condition (Figure adapted from HyIndoor Project [18])

ii. Two-vent mixing (Figure 3): A **stratified** regime for the two-opening case, one near the floor and one near the ceiling. Based on the Linden Model [22], a buoyant gas release in an enclosure with two ventilation openings is assumed to result in a displacement ventilation regime with the formation of an upper homogeneous concentration as shown in Figure 3 below. Similar to the one-vent model, two-vent model proposes a methodology to calculate the maximal concentration at steady-state. At steady state, the molar fraction, x_h in the upper layer is expressed by:

$$x_h = \frac{1}{C}\left(\frac{{Q_0}^2 h^{-5}}{g'}\right)^{1/3} \quad (3)$$

where, Q_0 is the release rate (m^3/s), C is a constant value, h is the interface height calculated based on the top and bottom vent areas, g' is reduced gravity $g' = g(\rho_{air} - \rho_{gas})/\rho_{air}$ (m/s^2), ρ_{air} and ρ_{gas} are density of the air and released gas, respectively, (kg/m^3).

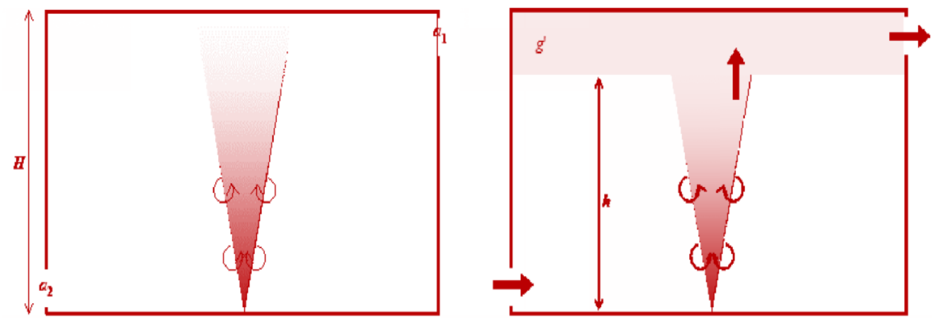

Figure 3 Idealised two-vent displacement ventilation scenario leading to a stratified gas distribution (Figure adapted from HyIndoor Project [18])

Jallais et al. [25] compared the results obtained by the Linden models to published and unpublished experimental results for helium and hydrogen releases and good agreement was observed for both cases. However, as mentioned by Molkov et al. [24], this was achieved by adjusting the discharge coefficient to a low 0.25 and provided that the basic hypothesis of the models is followed, i.e. leak is close to a plume at a level close to the floor and the vent configuration is similar.

Cariteau & Tkatschenko [23] amended the Linden equation for one-vent mixtures. This is applicable for natural ventilation, i.e. under the assumption of equal flows in and out of the enclosure, but not for passive ventilation, when the whole vent can be occupied by the gas released in the enclosure:

$$\bar{x}_h = \frac{Q_o^{2/3}}{(g(1-\rho_h/\rho_\alpha)k^2A^2d)^{1/3}} \quad (4)$$

The above equation was mentioned by Molkov et al. [24], who proposed an alternative model, i.e. **Molkov one-vent model**, in Eq.5, under the one-vent uniform mixing assumption. The comparison with experimental data showed a good correlation, towards the conservative side, with a deviation within about 20%. It was reported [24] that this comparison showed that this model can also be used in the case of stratification, as it is conservative;

$$X = f(X)\left[\frac{Q_o}{C_D A(g'H)^{1/2}}\right]^{2/3} \quad (5)$$

Where, X is the hydrogen volume fraction, Q_0 is the release rate (m^3/s), C_D is vent discharge coefficient, A is vent area (m^2), H is vent height (m), g' is reduced gravity $g' = g(\rho_{air} - \rho_{h_2})/\rho_{air}$ (m/s^2), ρ_{air} and ρ_{h_2} are density of the air and hydrogen, respectively, (kg/m^3) and function $f(X)$, which defines the difference between the approximate solution for volumetric fraction of hydrogen by natural ventilation, Eq.(2), and the exact solution of the problem by passive ventilation theory, Eq.6, is

$$f(X) = \left(\frac{9}{8}\right)^{1/3} \left\{ \left[1 - X \left(1 - \frac{\rho_{H_2}}{\rho_{air}} \right) \right]^{1/3} + (1 - X)^{2/3} \right\} \quad (6)$$

4.1 Vent discharge coefficient

The vent discharge coefficient C_D takes into account the energy loss due to turbulence that arise during the flow of the gas through the vent, i.e. C_D is used as a measure of vent flow resistance that accounts for the effective vent area through which pressurised gases are discharged with energy loss. Molkov et al. [24] that the dispersion model predictions of maximum concentration observed in the experiments had good agreement with the use of range of C_D varying from 0.60 to 0.95 (e.g. 0.60, 0.95 and 0.77 as average value of 0.60 and 0.90). Sensitivity study on the value of the vent discharge coefficient C_D is included in Section 5.3.

Further details of these models can be found in HyIndoor Guidelines report [18].

5. Validation of dispersion models

A number of analyses for varying parameters was undertaken to compare results between models as well as between models and experimental data. The following comparison studies are undertaken and presented in graphical form in the subsequent sections:

- Comparison of the Linden model [22] and the Molkov model [24]
- Benchmarking dispersion models with existing experimental data
- Comparison of dispersion models with Lot 2 and Lot 3 Programme of experiments within Work Package 7 (WP7) of the Hy4Heat project ([9], [10])

5.1 Comparison of the Linden model and Molkov model

5.1.1 One-vent models

One-vent models by **Linden et al.** [22] and **Molkov et al.** [24] are verified by using three arbitrary selected air tightness values, i.e. 3 $m^3/(hr/m^2)$, 5 $m^3/(hr/m^2)$, and 10 $m^3/(hr/m^2)$, representing typical sealed, moderate and leaky dwelling scenarios, respectively.

Air permeability rate 3 m3/(hr/m2)

Enclosure dimensions	W 3m x L 4m x H 3m
Permeability	3 $m^3/h/m^2$ (For the selected volume of the enclosure, this permeability rate corresponds to 0.12m^2 total vent area for H_2)
Pipe pressure	21 mbar
No. of vents	1
Model assumptions	Linden et al. [22] through Cariteau & Tkatschenko [23] formulation [1] Uniform mixture [2] Vent discharge coefficient 0.25
	Molkov et al. [24] 10. Uniform mixture 11. Vent discharge coefficient 0.6

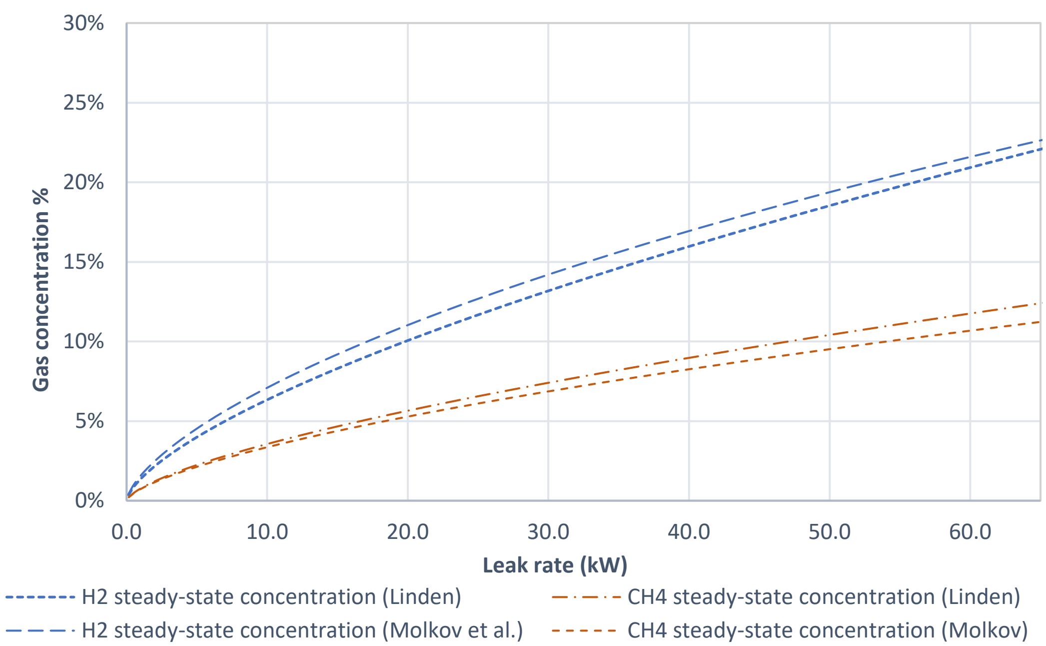

Figure 4: Steady state concentration of hydrogen and methane in a W 3m x L 4m x H 3m room with 1 vent calculated using phenomenological models by Linden et al. [22] and Molkov et al. [24] for leaks up to 64kW – air permeability 3 $m^3/h/m^2$.

Air permeability 5 m3/(hr/m2)

Enclosure dimensions	W 3m x L 4m x H 3m
Permeability	5 $m^3/h/m^2$ (For the selected volume of the enclosure, this permeability rate corresponds to $0.19m^2$ total vent area for H_2)
Pipe pressure	21 mbar
No. of vents	1
Model assumptions	Linden et al. [22] through Cariteau & Tkatschenko [23] formulation 12. Uniform mixture 13. Vent discharge coefficient 0.25
	Molkov et al. [24] 14. Uniform mixture 15. Vent discharge coefficient 0.6

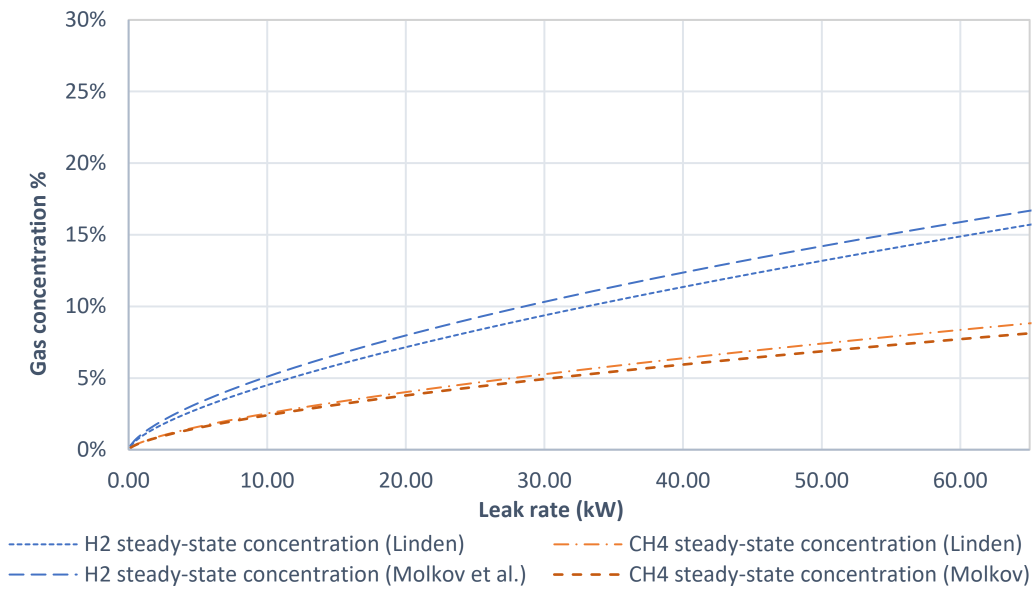

Figure 5: Steady state concentration of hydrogen and methane in a W 3m x L 4m x H 3m room with 1 vent calculated using phenomenological models by Linden et al. [22] and Molkov et al. [24] for leaks up to 64kW – air permeability 5 $m^3/h/m^2$.

Air permeability 10 m3/(hr/m2)

Enclosure dimensions	W 3m x L 4m x H 3m
Permeability	10 $m^3/h/m^2$ (For the selected volume of the enclosure, this permeability rate corresponds to 0.32m^2 total vent area for H_2)
Pipe pressure	21 mbar
No. of vents	1
Model assumptions	Linden et al. [22] through Cariteau & Tkatschenko [23] formulation 16. Uniform mixture 17. Vent discharge coefficient 0.25
	Molkov et al. [24] 18. Uniform mixture 19. Vent discharge coefficient 0.6

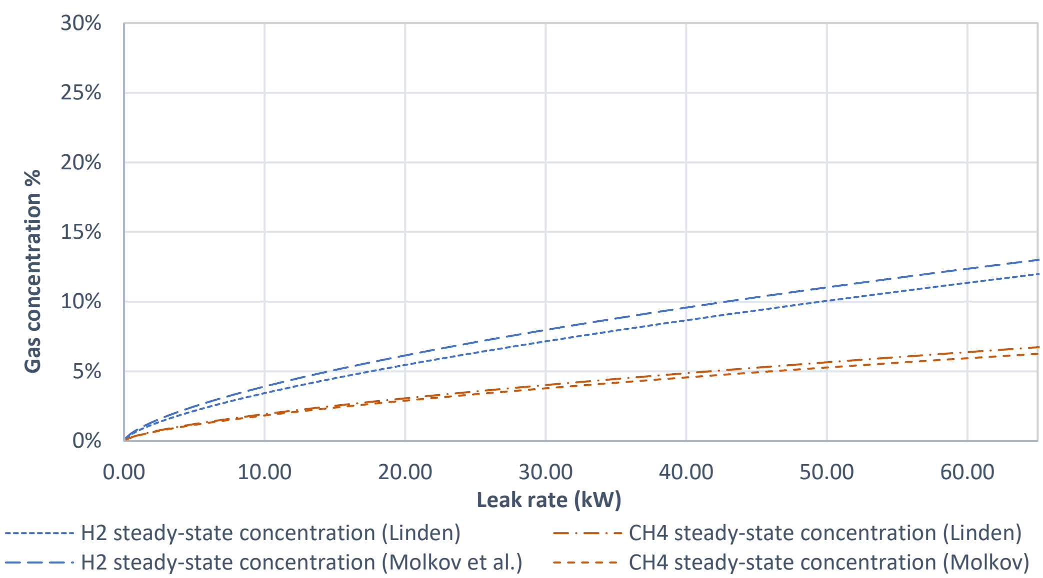

Figure 6: Steady state concentration of hydrogen and methane in a W 3m x L 4m x H 3m room with 1 vent calculated using phenomenological models by Linden et al. [22] and Molkov et al. [24] for leaks up to 64kW – air permeability 10 $m^3/h/m^2$.

5.1.2 Two-vent model (Linden model only) for hydrogen and methane

Air permeability 3 m3/(hr/m2)

Enclosure dimensions	W 3m x L 4m x H 3m
Permeability	3 $m^3/h/m^2$ Assuming same equivalent total vent area as in the one-vent model (i.e. 0.12m^2 total vent area for H_2, with 0.06m^2 vent area located at bottom and top of the enclosure)
Pipe pressure	21 mbar
No. of vents	2
Model assumptions	Linden et al. [22] 20. Stratified conditions 21. Bottom & top vent discharge coefficient 0.5 22. Height up to mid of top vent 2m

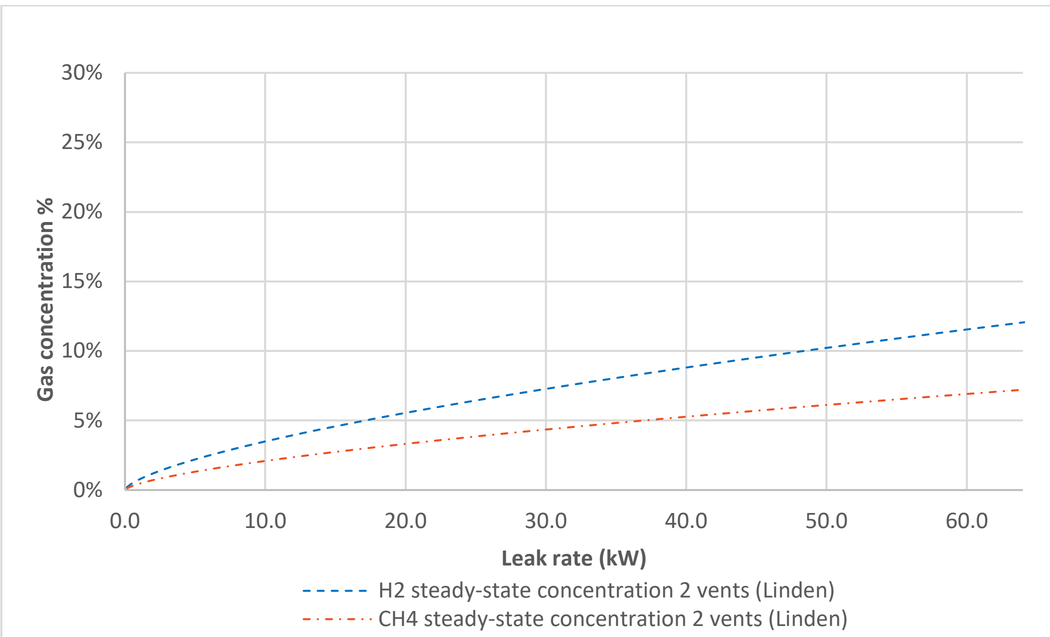

Figure 7 Steady state peak concentration of hydrogen and methane in the top layer of a W 3m x L 4m x H 3m room with 2 vents calculated using phenomenological model by Linden et al. [22] for leaks up to 64kW – air permeability 3 $m^3/h/m^2$.

Air permeability 5 m3/(hr/m2)

Enclosure dimensions	W 3m x L 4m x H 3m
Permeability	5 $m^3/h/m^2$ Assuming same equivalent total vent area as in the one-vent model (i.e. 0.19m^2 total vent area for H_2, with 0.095m^2 vent area located at bottom and top of the enclosure)
Pipe pressure	21 mbar
No. of vents	2
Model assumptions	Linden et al. [22] 1. Stratified conditions 2. Bottom & top vent discharge coefficient 0.5 3. Height up to mid of top vent 2m

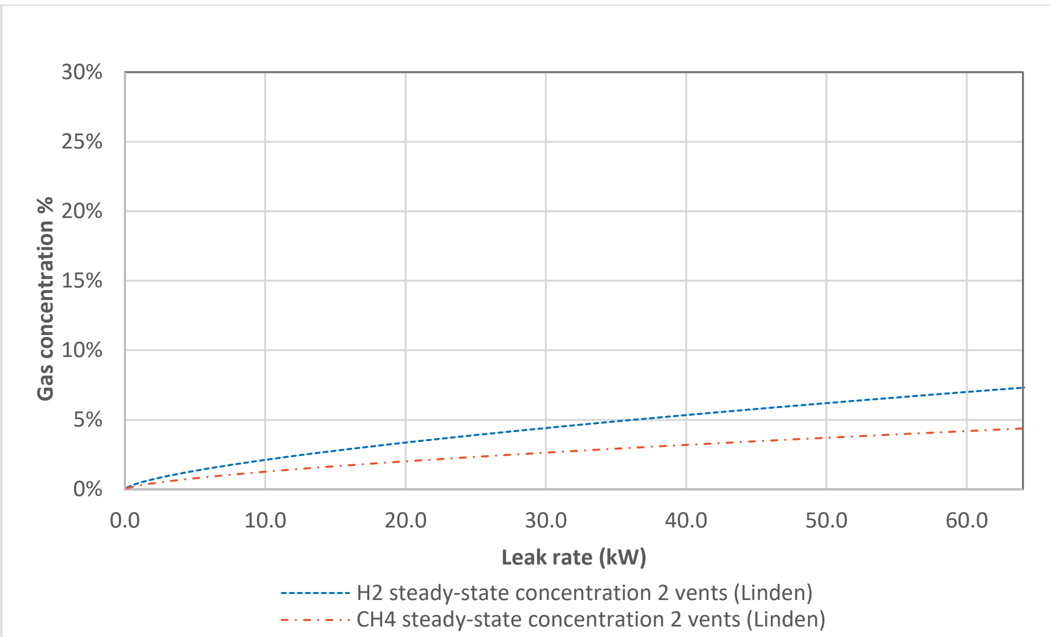

Figure 8 Steady state peak concentration of hydrogen and methane in the top layer of a W 3m x L 4m x H 3m room with 2 vents calculated using phenomenological model by Linden et al. [22] for leaks up to 64kW – air permeability 5 $m^3/h/m^2$.

Air permeability 10 m3/(hr/m2)

Enclosure dimensions	W 3m x L 4m x H 3m
Permeability	10 $m^3/h/m^2$ Assuming same equivalent total vent area as in the one-vent model (i.e. 0.32m^2 total vent area for H_2, with 0.16m^2 vent area located at bottom and top of the enclosure)
Pipe pressure	21 mbar
No. of vents	2
Model assumptions	Linden et al. [22] 23. Stratified conditions 24. Bottom & top vent discharge coefficient 0.5 25. Height up to mid of top vent 2m

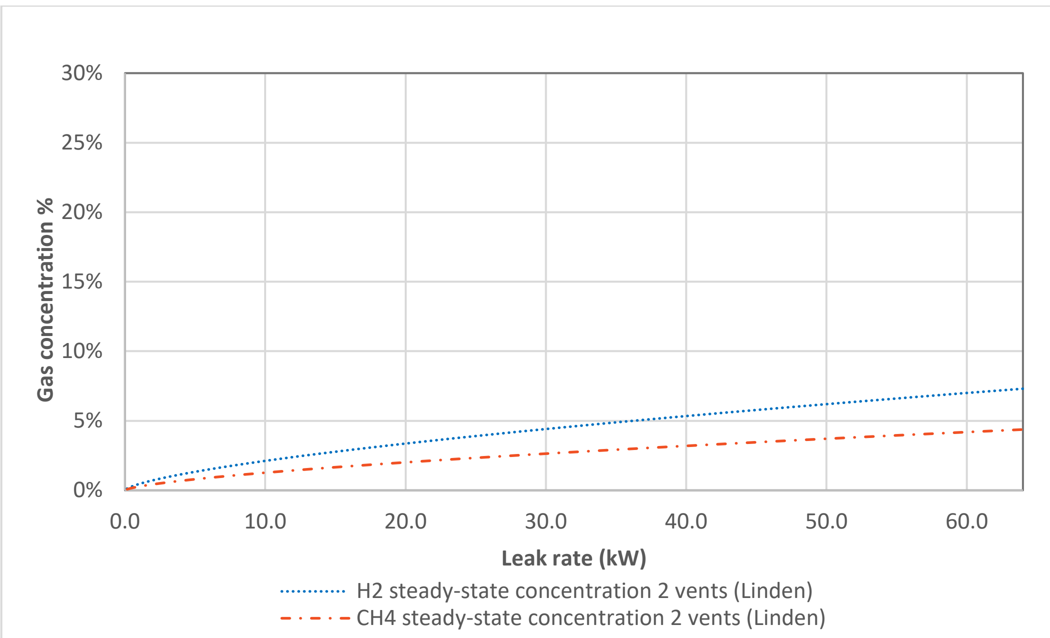

Figure 9: Steady state peak concentration of hydrogen and methane in the top layer of a W 3m x L 4m x H 3m room with 2 vents calculated using phenomenological model by Linden et al. [22] for leaks up to 64kW – air permeability 10 $m^3/h/m^2$.

5.1.3 Summary of model comparison

For small to moderate leaks, there is a good agreement between the two models, i.e. Linden model and Molkov model used for the uniform mixing case with a single vent. For larger leaks, however, results tend to differ significantly as can be seen in Figure 10 below, leading up to a significant gap for a full-bore leak, assuming a 30mm diameter pipe for the same discharge coefficient. However, it is expected that the leak flow rate of H2 above approximately 64kW (corresponding to ~8mm leak hole size) would not be sustained by the network. Therefore, the QRA will consider an appropriate low frequency for these larger leak rates.

Figure 11 below shows the leak hole diameters corresponding to H2 leak flow rates presented in Figure 10.

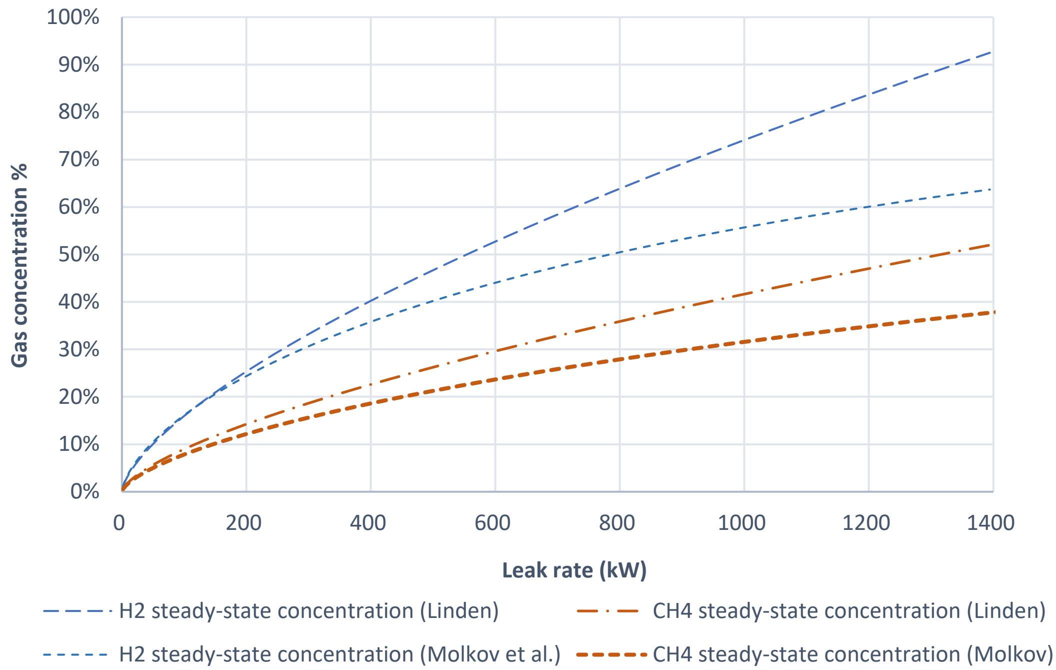

Figure 10: Steady state concentration of hydrogen and methane in a W 3m x L 4m x H 3m room calculated using phenomenological models by Linden et al. [22] and Molkov et al. [24] for leaks corresponding to leak hole sizes up to 30mm (corresponding to H_2 leak flow rate of 1400kW) from a pipe at 21mbar internal pressure – air permeability 3 $m^3/h/m^2$

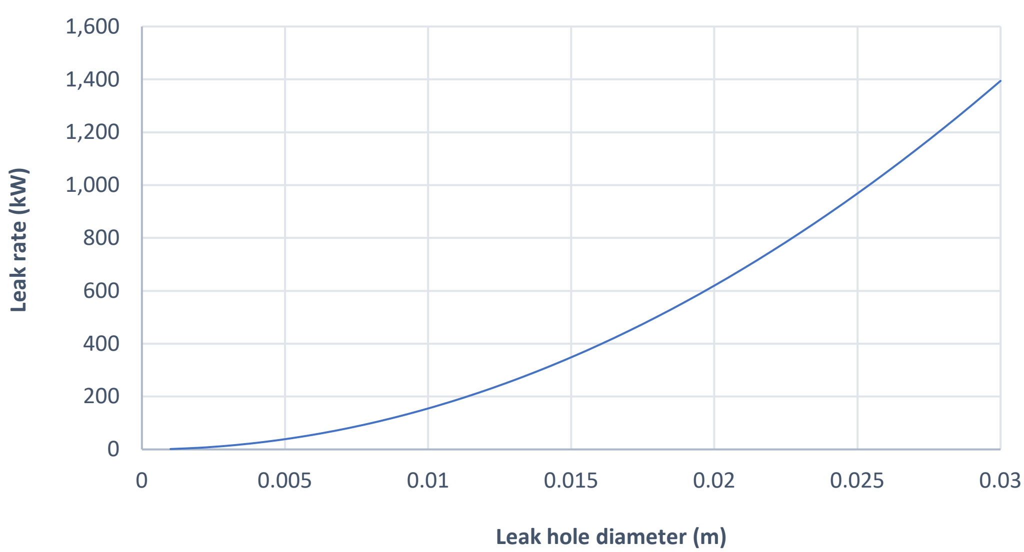

Figure 11: H_2 leak flow rate vs. leak hole diameter

5.2 Benchmarking dispersion models with existing data

To obtain confidence in the modelling equations used for dispersion assessment, Linden model and Molkov model are compared with experimental data obtained from literature. For benchmarking, two cases of vent configurations are considered: (1) one-vent configurations and (2) two-vent configurations.

A list of experimental studies used for analytical model validation on helium and hydrogen is provided in Table 2. It is important to note that since helium is not flammable and is the gas with the most similar features and behaviour to hydrogen regarding the dispersion properties, helium is often used as a substitute for hydrogen in experimental studies of hydrogen release.

Further comparison studies for Linden model and Molkov model can be found in Jallias et. al. [25].

Table 2: Summary of the experiments used for model verification

Gas release in a one-vent enclosure	
Experiments used for verification	CEA GARAGE Experiments Cariteau et al. [26]
Gas release in a two-vent enclosure	
Experiments used for verification	CEA GARAGE Experiments Cariteau et al. [26] Barley & Gawlick [27]

5.2.1 Experimental data with one-vent configurations

The dispersion results from Linden model and Molkov model for one-vent configurations were compared to the CEA Garage experimental measurements by Cariteau et al. [26]. Inside the tightly sealed enclosure of W2.96 x L5.76 x H2.42 m, helium dispersion experiments were performed with a vent of 200mm diameter located 2.22m above the floor. The height of the enclosure was 2.42m. The initial condition of this enclosure was full of steady air and helium gas was injected through 70mm diameter vertical nozzle which exited 0.2m above the floor.

Table 3: CEA GARAGE Experiments – Cariteau et al. [26]

Experiment	
Enclosure	CEA GARAGE W2.96 x L5.76 x H2.42 m
Gas used	Helium
Vent	1 circular vent d=0.2m at 2.22m from the floor
Leak	1. 70mm nozzle at 0.2m from the floor 2. Leak rates from 0.1Nl/min to 18Nl/min
Calculation	
Model assumptions	Linden et al. [22] through Cariteau & Tkatschenko [23] formulation 3. Uniform mixture 4. Vent discharge coefficient 0.25
	Molkov et al. [24] 5. Uniform mixture 6. Vent discharge coefficient 0.6

Figure 12 compares the simplified dispersion model results with flow rates ranging from 1.2x10-4 to 3.3x10-4 m3 /s to experimental data from Cariteau et al. [21] and it is found that the difference is within a margin of about 2%. Figure 12 also validates that both of the one-vent model developed by Linden et al. [22] and Molkov et al. [24] can be applied to these scenarios.

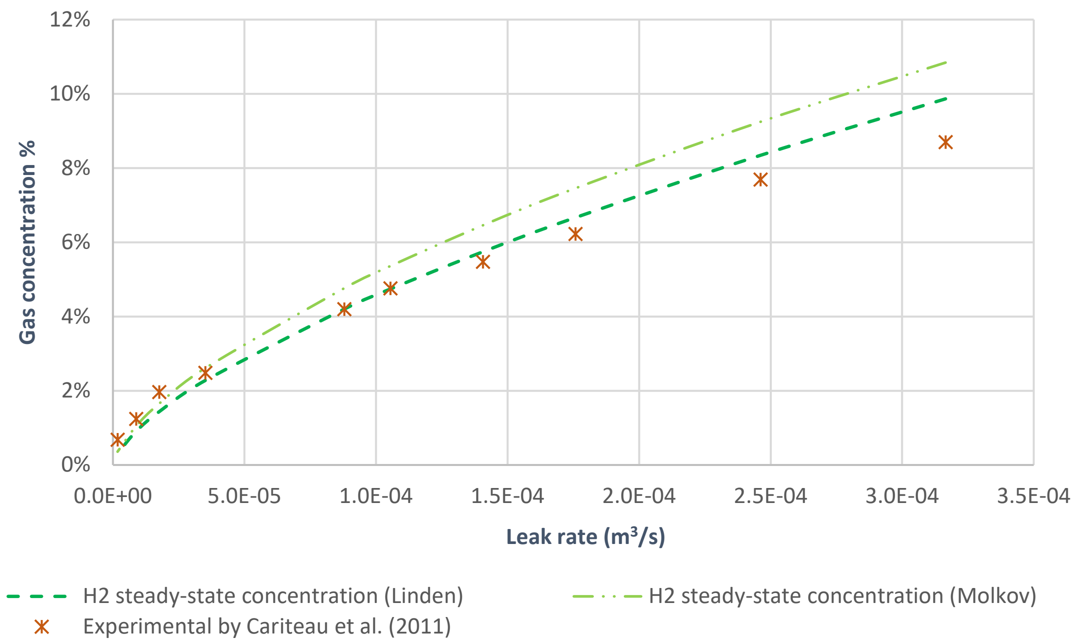

Figure 12: Comparison of analytical results for helium from Linden (1999) and experimental results from Cariteau et al. [26]

5.2.2 Experimental data with two-vent configurations

Experiments were performed with helium release in the CEA GARAGE facility (L5.76 x W2.96 x H2.42 m) [21]. The garage is equipped with two circular vents (0.2 m diameter) located at 0.22 and 2.22 m from the floor. Helium is released by a 70 mm diameter orifice at 0.20 m from the floor. With the vent location and size, a homogeneous layer is calculated at 0.93 m above the floor. Details of these experiments and assumed coefficients for the analytical models are summarised in Table 4.

Table 4: CEA GARAGE Experiments – Cariteau et al. [26]

Experiment	
Enclosure	CEA GARAGE L5.76 x W2.96 x H2.42 m
Gas used	Helium
Vents	2 circular vents d=0.2m at 0.22m and 2.22m from the floor
Leak	7. 70mm nozzle at 0.2m from the floor
Calculation	
Model assumptions	Linden et al. [22] 8. Stratified conditions 9. Bottom & top vent discharge coefficient 0.50

As shown in Figure 13, a good agreement between calculations and experiments is obtained.

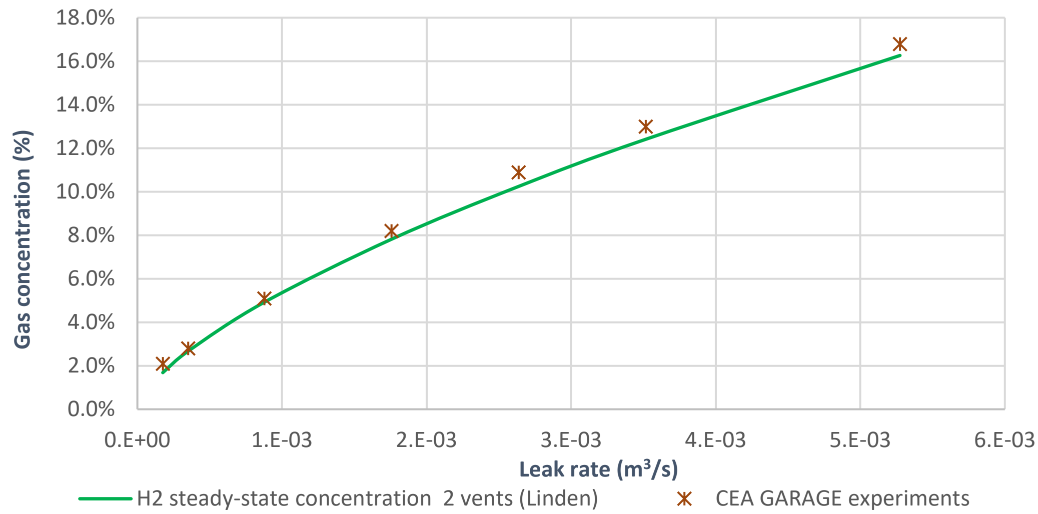

Figure 13: Comparison between analytical results from Linden (1999) for 2 vents configuration and experimental results from experiments performed for CEA GARAGE study

Barley and Gawlick [27] also performed helium release experiments in a rectangular room (L7.02 x W4.29 x H2.74 m). This room is placed in a big hall avoiding wind effects. The lower and upper ventilation openings (W32.4 x H24.3 cm) are located at 0.37 and 2.38 m from floor, on the same wall. The leak was located at variable height above the centre of the test room floor (varying from 0.61m to 1.22m). The injection system is a local diffuser (automobile oil filter element, 9.6-cm height and 8-cm diameter) or a line diffuser (1.83-m length porous hose). These configurations are summarised in Table 5.

Table 5: Barley and Gawlick [27]

Experiment	
Enclosure	L7.02 x W4.29 x H2.74 m
Gas used	Helium
Vents	W32.4 x H24.3 cm at 0.37m and 2.38 m from floor, on the same wall
Leak	10. Local diffuser, h=9.6 cm and d=8 cm (P) 11. Line diffuser, 1.83 m long porous hose (L) 12. Varying heights above floor
Calculation	
Model assumptions	Linden et al. [22] 13. Stratified conditions 14. Bottom & top vent discharge coefficient 0.50

As shown in Figure 14, a rather good agreement is obtained between modelling and experiments even if the calculated results are below experiment values. It is important to note that increasing the height of the leak source leads to an increase in the maximum concentration recorded in the experiments. This shows that when the release location is not close to the floor level, the model predictions are not accurate.

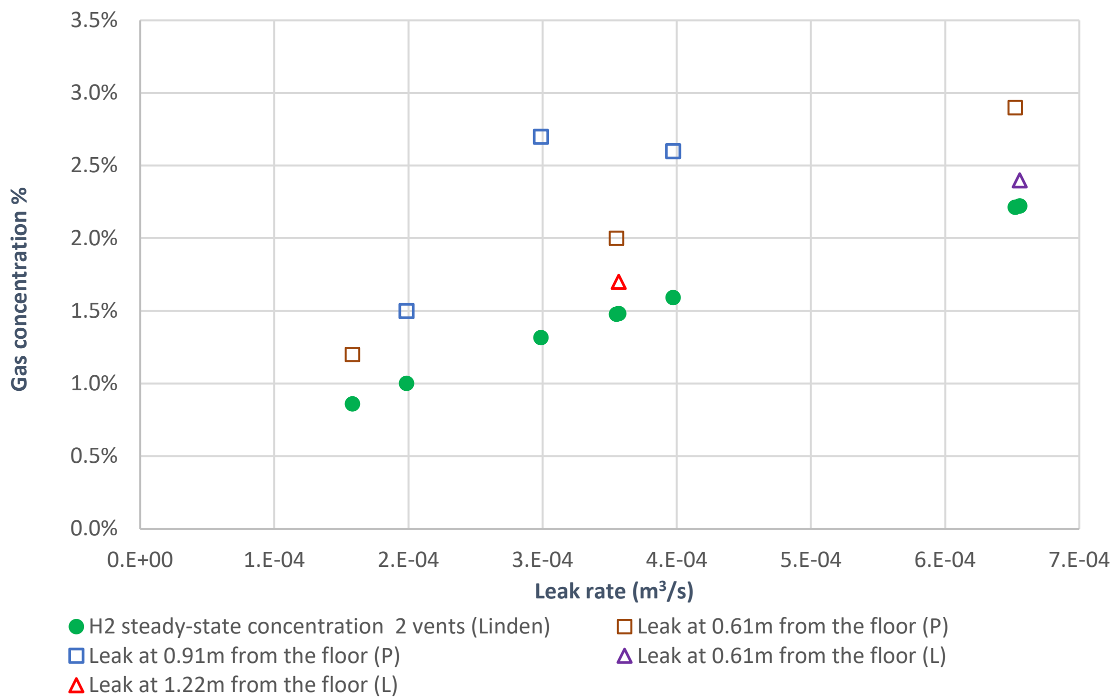

Figure 14: Comparison between analytical results from Linden et al. [22] for 2 vents configuration and experimental results by Barley & Gawlick [27] for varying height of leak location.

5.2.3 Conclusions

For enclosures with a one-vent configuration, it is observed that a well-mixed regime is formed. The comparison study showed a good agreement between calculations with one-vent models developed by Linden et al. [22] and Molkov et al. [24] and recently published experiments.

For hydrogen release in an enclosure with two-vents, formation of a homogeneous upper layer is observed. Modelling this with Linden model with two-vent configuration showed good agreement with the recently published experiments with an enclosure which is naturally ventilated with two openings without wind.

Further modelling and experiments comparisons in steady state conditions can be found in Jallias et al. [25].

5.3 WP7 Lot 2 and Lot 3 test comparison

In this section comparisons are performed between the dispersion model predictions for concentration build-up and the experimental data obtained from Lot 2 and Lot 3 programme of works within Work Package 7 (WP7) of the Hy4Heat project. This comparison study aimed to compare the steady-state build-up for both hydrogen and methane (natural gas) in a typical domestic property.

In order to examine the dispersion of hydrogen and understand how its steady-state concentration compares to methane, experiments were conducted by DNV GL to measure hydrogen accumulation and distribution levels within confined spaces in a typical domestic property. The experiment setup was designed with two major objectives: first, simulating realistic leak events in a typical domestic property, and second, keeping experiment relatively simple to provide accumulation and distribution data for hydrogen and methane gas considering a range of property sealing conditions (i.e. doors closed or open) and release sizes into (i) kitchen cupboards and inset meter box for Lot 2 programme; and (ii) basement and kitchen boiler cupboard for Lot 3 programme. Therefore, the programme of Lot 2 and Lot 3 experiments was carried out with a range of hydrogen and methane release rates and sealing / vent configurations to generate concentration data that can be used to validate analytical models.

Table 6 summarises the experimental arrangements for Lot 2 and Lot 3 programme and further details of the test plan, properties of the test environment, instrumentation, experimental procedure and data collection and are included in DNV GL's WP7 reports ([15] and [16]).

Table 6: Summary of Lot 2 and Lot 3 experimental arrangements

Variables	**Lot 2**	**Lot 3**
Description	Cupboard level leakage and accumulation data	Property level leakage and accumulation data
Fuel	Methane (CH_4) Hydrogen (H_2)	Methane (CH_4) Hydrogen (H_2)
Number of tests	74	102
Hole size (mm)	0.6, 0.9, 1.8, 2.5, 3.6, 5.1, 7.2	5, 10, 15 (nominal)
Release rates (m^3/h)	H_2: 0.13 to 18.4 CH_4: 0.04 to 6.4	H_2: 4.5 to 79 CH_4: 1.6 to 28
Location	Kitchen – different cupboards & Meter box	Basement & Kitchen boiler cupboard
Sealing conditions	Cupboard and kitchen doors closed, but not sealed with tape. Utility and living room doors open Basement of the house: fully sealed. Fireplace in the living room: fully sealed	Kitchen and / or Basement door open or closed
Aim	Produce data for release in small enclosed spaces (i.e. cupboards) to investigate the subsequent effect on wider room	Produce data for release in basement or kitchen boiler cupboard to investigate the subsequent effect on wider rooms with open and closed house doors

Available experimental data collected within the WP7 Lot 2 and Lot 3 programme of Hy4Heat ([15] and [16]) were performed for mostly leaks up to 15mm leak hole size. Table 7 below lists a summary calculated leak flow rate values used in the dispersion model corresponding to the leak hole sizes up to 15mm. For all leak flow calculations, leak discharge coefficient of 0.6 is used.

In order to understand the sensitivity to different values of vent discharge coefficient C_D, comparison study of peak measured CH_4 and H_2 concentrations recorded in the kitchen when door is closed and predictions by Linden one-vent, Molkov one-vent and Linden two-vent models is undertaken. Figure 15 and Figure 17 show the comparison of models with the data for CH_4 and H_2, respectively when the vent discharge coefficient C_D = 0.60 is applied to all models. This comparison demonstrates that predictions by Molkov one-vent model have a good fit with the experimental data with C_D = 0.6.

Figure 16 and Figure 18 compare the experimental results for the same tests with the predictions by Molkov one-vent model using different vent discharge coefficients, where C_D = 0.60, 0.77 (average of 0.6 and 095) and 0.95. This comparison demonstrates that the predictions by Molkov one-vent model with vent discharge coefficient value of $C_D = 0.60$ are in closer agreement with the measured data. Therefore, Molkov one-vent model with vent discharge coefficient value of $C_D = 0.60$ is used for the rest of the comparison study between the dispersion model predictions for concentration build-up and the experimental data obtained from Lot 2 and Lot 3 programme.

Table 7: Leak flow rate, Q_o (m^3/h) values for H_2 and CH_4 corresponding to different leak hole sizes (used in the dispersion model)

Hole diameter (mm)	**Leak flow rate Qo (m3/h) for H2**	**Leak rate (m3/h) Qo for CH4**
0.3	0.03	0.01
0.6	0.13	0.05
0.9	0.30	0.10
1.2	0.53	0.19
1.8	1.18	0.42
2.5	2.28	0.81
2.8	2.87	1.01
3.55	4.61	1.63
4.14	6.26	2.21
4.92	8.85	3.12
5.1	9.51	3.35
5.8	12.29	4.34
6.97	17.75	6.26
7.2	18.94	6.68
7.6	21.11	7.45
8.29	25.11	8.86
8.8	28.30	9.99
9.76	34.81	12.28
10	36.54	12.89
10.6	41.06	14.49
11.2	45.84	16.17
11.8	50.88	17.95
12.4	56.19	19.83
13	61.76	21.79
13.6	67.59	23.85
14.08	72.45	25.56
14.61	78.00	27.52
14.7	78.97	27.86
15	82.22	29.01

For the validation study of the dispersion models and identification of the air permeability rates for each confined space with different sealing conditions (e.g. doors open / closed), experiments are grouped based on the leak locations and sealing conditions so that comparisons can be modelled for kitchen, living room, basement and cupboard as summarised in Table 8.

Lot 2 tests were performed to understand the gas build-up at steady-state condition when there is a leak in a small enclosed space (i.e. kitchen cupboards) and subsequent effect on wider room. These tests were conducted with cupboard and kitchen doors closed, therefore, dispersion model is used to estimate the hydrogen and methane gas concentration build-up in the kitchen, where the leak source is located, i.e. kitchen cupboards. Lot 2 tests included release scenarios where leaks occurred into an inset meter cupboard on the external wall of the domestic property (Experimental IDs L2-003:L2-008 an L2-043:L2-048). As the cupboard sample points to record the data were located either within the meter box or within the cavity wall with a release into the cavity wall rather than directly to the house rooms, these tests were not included in this comparison study.

Lot 3 tests provided data for the release locations either at the basement or kitchen boiler cupboard. These data provided insights of the concentrations and air permeability rates in a larger confined space (i.e. in basement) when basement doors are open or closed. Additionally, Lot 3 test data is also used to understand the effect of concentration build-up in the kitchen when the kitchen door is closed or open.

Figure 19 through Figure 30 present the experimental and dispersion model results for one-vent configuration for kitchen, living room, basement and cupboard enclosures. For these comparisons, one-vent Molkov model is included in this report, but similar results are also obtained with the use of one-vent Linden model. Also, a representation of hydrogen and methane concentration distributions along the height of the floor level (e.g. low-level, mid-level and high-level) are presented in Figure 31 and Figure 32 for kitchen using the corresponding experimental data using and comparisons are made with the predictions by one-vent and two-vents dispersion models. The observations from these figures are presented in the subsequent sections.

5.3.1 Lot 2 and Lot 3 experimental results and discussions

Postprocessing of the experimental results allowed visualisation of the measured concentrations of hydrogen and methane over the height of the room and provided observations on the following:

1. According to the experimental data, at steady state, maximum recorded hydrogen concentrations increase with the increased hydrogen flow rate. Similar observation is valid for methane with relatively less increase in the peak concentrations.

2. The maximum concentration of hydrogen significantly increases with the height of the leak release location. This can be observed by comparing the concentrations resulted due to the leak release from kitchen wall cupboard with the values recorded from the tests when the leak was originated from kitchen base cupboard and undersink cupboard in Lot 2 and Lot 3 experiments (Figure 15 and Figure 16). This experimental information highlights the importance of considering release height and its distance to the ceiling level when this information is available.

3. The height of leak has also an influence on the vertical distribution regimes, i.e. stratification was identified for the experiments for hydrogen, where the concentrations at the floor level (i.e. kitchen-low) and mid-level were significantly lower than the maximum concentrations at the high-level when the leak was close to the ceiling, i.e. from kitchen wall cupboard as shown in Figure 31. On the other hand, for methane, Figure 32 shows that vertical distribution regime was identified as two-layer regime, where the concentration values at the high- and mid-level of the kitchen were close to each other, whereas the measurement from the floor-level was approximately one-third to half of the maximum concentration.

4. Influence of ventilation:
   a. Experimental investigations for kitchen (i.e. Experiment ID L2-062A, L2-063A, L2-064A with leak from kitchen base cupboard) showed that if the kitchen was vented above the doors, hydrogen concentration was reduced by up to 12% change in percentage points. This is demonstrated in Figure 33.
   b. It is observed that in vented scenarios (Experiment ID L3-037A, L3-085A for methane and hydrogen resulting from a leak in the kitchen boiler cupboard, respectively), reduction in methane concentration was more than hydrogen as shown in Figure 34.
   c. In light of the findings of the vent tests, additional 31 tests conducted within WP7 to further investigate the effect of additional wall vents. These additional test with added vents ceiling vents ducted through external wall or cupboard walls showed that additional vent reduced the maximum concentration within the room of release and also lower the gas inventory within the whole whose.

Additional experimental data assessment is included in Kiwa [7] with the aim to better understand the hydrogen and methane accumulation and mixing processes.

5.3.2 Dispersion model validation and discussions

The following conclusions have been obtained from the theoretical model validation with the WP7 experimental data:

1. Overall, the Linden model and Molkov model appear to provide reasonable predictions of most experiments. One notable exception is the experiments with high-release locations, such as release from kitchen wall cupboard (Lot 2) and kitchen boiler cupboard (Lot 3) as shown in Figure 19,and Figure 21, for hydrogen and Figure 20 and Figure 22 for methane. In these experiments, release locations are high above the floor level and there is a reduced gap between the cupboards and ceiling, resulting in more stratified concentrations. This observation highlights the importance of considering release height and its distance to the ceiling when this information is available.
2. In some of the experiments when the door of the kitchen is open the agreement with the measurements and the dispersion models is rather inconsistent as shown in Figure 21 and Figure 22 which is due to the fact that the vent through the door is modelled as a single large vent for the different release locations: (i) basement release, (ii) kitchen boiler cupboard release, which are resulting from a release at the floor level and close to the ceiling, respectively, hence the data also differ significantly.
3. Overall, most of the peak concentrations are over-estimated for hydrogen and under-estimated for methane with dispersion models, which is preferred as a conservative approach for the purpose of relative consequence assessment between hydrogen and methane, because the results of the dispersion model will be used in Hy4Heat QRA consequence assessment and a dispersion event at a higher concentration for a given leak flow rate will potentially produce worse consequences for hydrogen than methane.
4. Simplified methods can be used to estimate the concentration reached in an enclosure in case of accidental leak, provided that the main assumptions of the models are valid:
   a. The leak is at a level close to the floor: For height of release close to ceiling, reduced agreement is observed between the theoretical results and experiments.

b. The leak rate is low, i.e. the leak hole diameter < ~ 10mm

Generally, the results obtained through analytical models showed good agreement with the experimental data leading to the conclusion that the dispersion models can be effectively used to support consequence assessment procedures and QRA framework concerning dispersion scenarios.

Where the models underestimate the stratification, combination of dispersion model and experimental data is suggested for the consequence assessment. Using the estimated height of the peak layer obtained from two-vent model and the observations of the outputs from the WP7 Lot 2 and Lot 3 experiments, the consequence model considered the stratification of hydrogen (and methane) by assuming the "equivalent volume" of hydrogen (and methane) contributing to the confined combustible vapour cloud explosion, rather than assuming that entire volume of the enclosure is filled with the peak concentration values obtained from the simplified models. It is also suggested to directly utilise the WP7 Lot 2 and Lot 3 peak concentration data, where the models underestimate the peak concentrations. Further details on the consideration of stratification in the consequence modelling can be found in WP7 Risk assessment: Consequence modelling report [11].

Table 8: WP7 Lot 2 and Lot 3 experiments used for the comparison study of dispersion models

Experiment ID		**Leak Location**	**Sealing**	**Dispersion model**	**Figure reference**	
CH_4	**H_2**				**CH_4**	**H_2**
L2-010:L2-016	L2-050:L2-056	Kitchen wall cupboard[1]	Cupboard door, closed, All doors closed	Kitchen concentration – door closed	Figure 15 [2]	Figure 17 [2]
L2-018:L2-024	L2-058:L2-064	Kitchen base cupboard			Figure 16 [2]	Figure 18 [2]
L2-026:L2-032	L2-066:L2-072	Kitchen behind base cupboard			Figure 19	Figure 20
L2-034:L2-040	L2-074:L2-082	Kitchen under sink cupboard				
L3-033:L3-040	L3-081:L3-088	Kitchen boiler cupboard[1]				
L3-025:L3-032	L3-073:L3-080	Basement high – Downwards release	All doors open	Kitchen concentration – door open	Figure 21	Figure 22
L3-041:L3-048	L3-089:L3-096	Kitchen boiler cupboard[1]				
L3-025:L3-032	L3-073:L3-080	Basement high		Living room concentration – door open	Figure 23	Figure 24
L3-041:L3-048	L3-089:L3-096	Kitchen boiler cupboard[1]				
L3-001:L3-008	L3-049:L3-056	Basement high – Upwards release[1]	Basement door closed	Basement concentration – door closed	Figure 25	Figure 26

[1] Release location high from floor level

[2] Figures show comparison between maximum measures CH4 and H2 concentrations in kitchen and predictions by Linden one-vent, Molkov one-vent, and Linden two-vent models with different vent discharge coefficients, C_D

Experiment ID		Leak Location	Sealing	Dispersion model	Figure reference	
CH_4	H_2				CH_4	H_2
L3-009:L3-016	L3-057:L3-064	Basement high – Downwards release[1]				
L3-017:L3-024	L3-065:L3-072	Basement high – Horizontal release[1]				
L2-018:L2-024	L2-058:L2-064	Kitchen base cupboard	Cupboard door, closed, All doors closed	Cupboard concentration – door closed	Figure 27	Figure 28
L2-026:L2-032	L2-066:L2-072	Kitchen behind base cupboard				
L2-034:L2-040	L2-074:L2-082	Kitchen under sink cupboard				
-	L2-062A,063A,064A L3-081A,083A,085A	Kitchen base cupboard[3] Kitchen boiler cupboard[4]	Cupboard door, closed, All doors closed, vent above the kitchen door	Kitchen concentration – door closed, kitchen ventilation	-	Figure 29
-	L2-064B	Kitchen base cupboard[3]	Cupboard door, closed, All doors closed, vent on the sides of cupboard	Cupboard concentration – door closed, cupboard ventilation	-	Figure 30

[3] Vent case validated only for hydrogen

[4] Vent case validated only for hydrogen

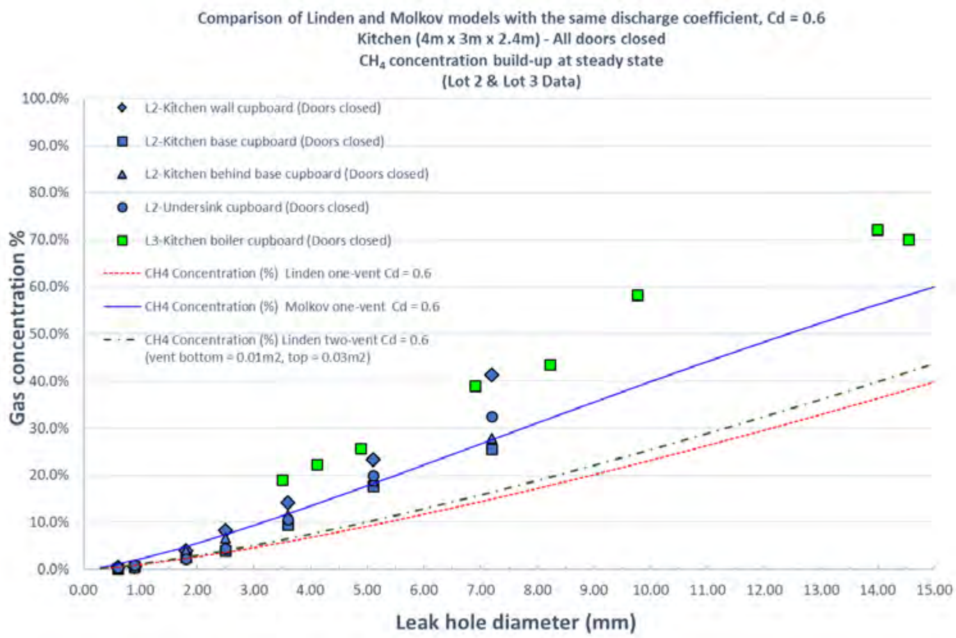

Figure 15: Comparison of predictions by Linden one-vent model, Molkov one-vent model and Linden two-vent model with the same vent discharge coefficient, $C_D = 0.6$ with measured peak CH_4 concentrations in kitchen resulting from cupboard releases (doors closed, assumed total leak and vent area = $0.04m^2$)

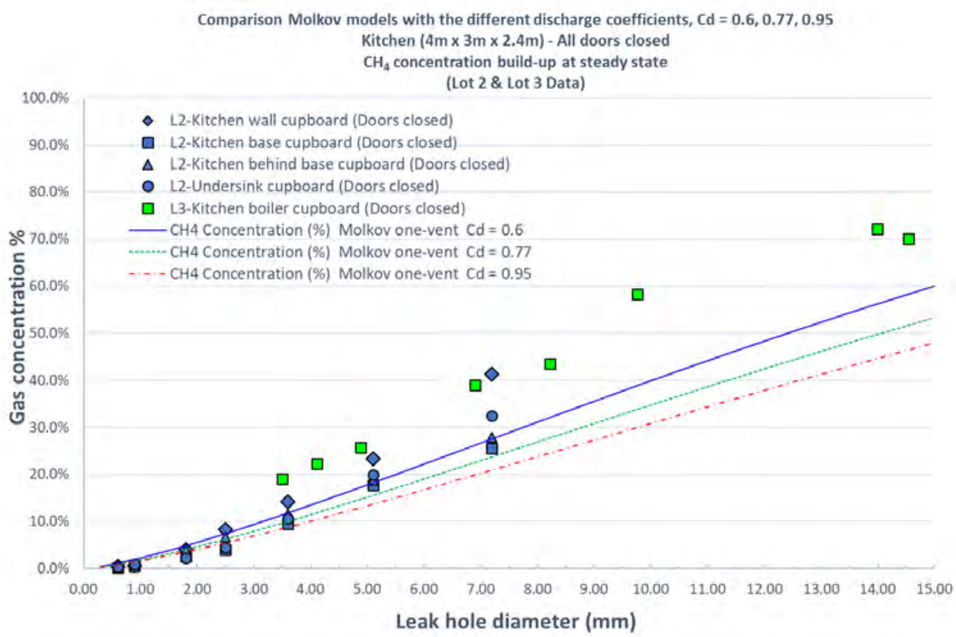

Figure 16: Comparison of predictions by Molkov one-vent model with the different vent discharge coefficients, $C_D = 0.6$, 0.77 and 0.95 with measured peak CH_4 concentrations in kitchen resulting from cupboard releases (doors closed, assumed total leak and vent area = $0.04m^2$)

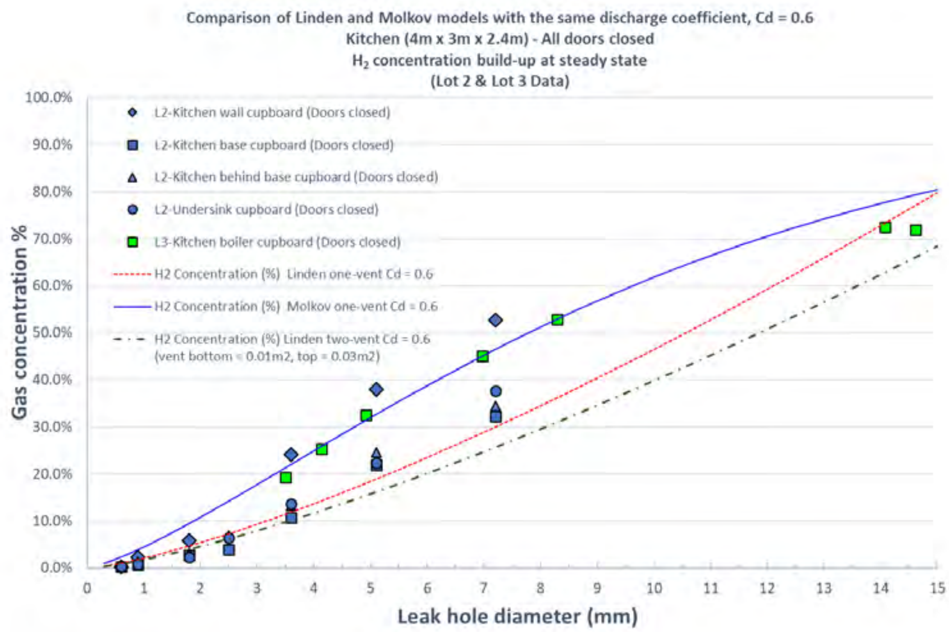

Figure 17: Comparison of predictions by Linden one-vent model, Molkov one-vent model and Linden two-vent model with the same vent discharge coefficient, C_D = 0.6 with measured peak H_2concentrations in kitchen resulting from cupboard releases (doors closed, assumed total leak and vent area = 0.04m^2)

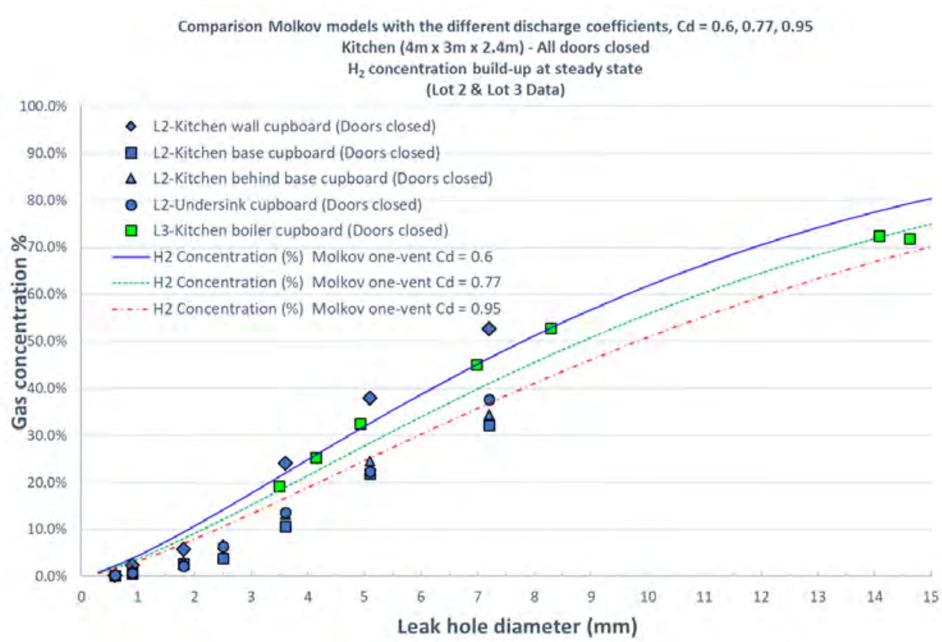

Figure 18: Comparison of predictions by Molkov one-vent model with the different vent discharge coefficients, C_D = 0.6, 0.77 and 0.95 with measured peak H_2 concentrations in kitchen resulting from cupboard releases (doors closed, assumed total leak and vent area = 0.04m^2)

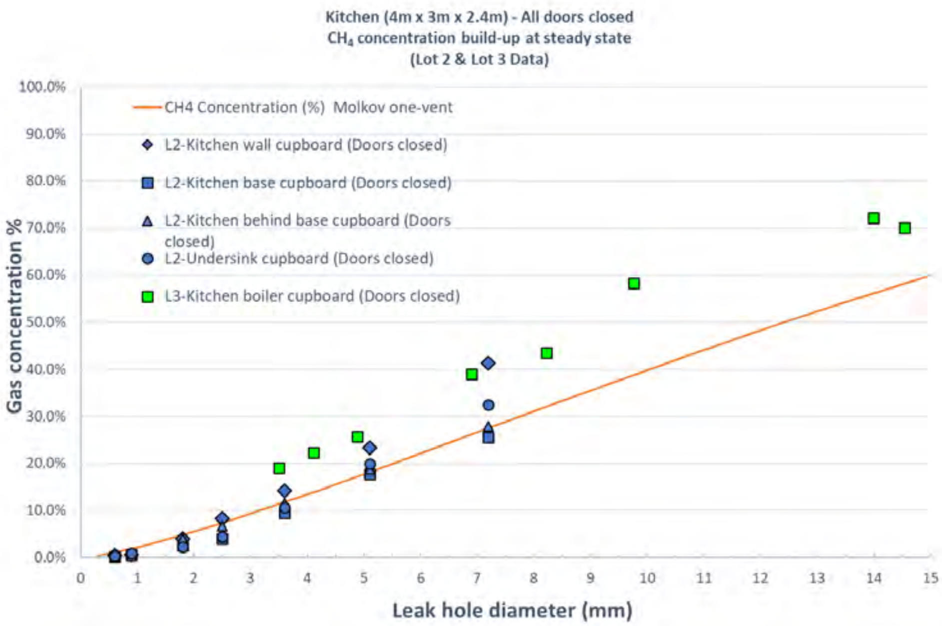

Figure 19: Comparison of predicted and measured peak CH_4 concentrations in kitchen resulting from cupboard releases (doors closed, assumed total leak and vent area = $0.04m^2$)

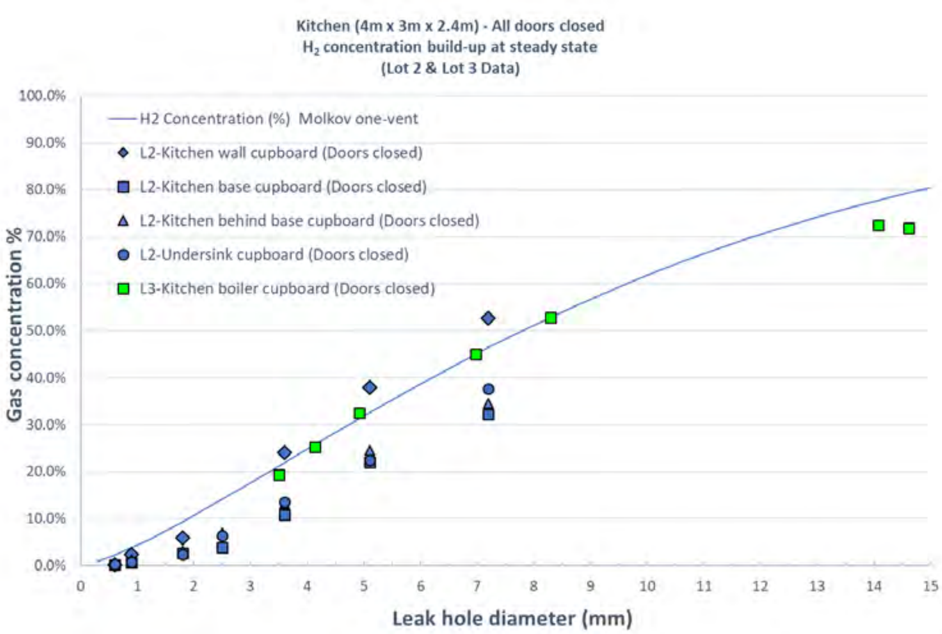

Figure 20: Comparison of predicted and measured peak H_2 concentrations in kitchen resulting from cupboard releases (doors closed, assumed total leak and vent area = $0.04m^2$)

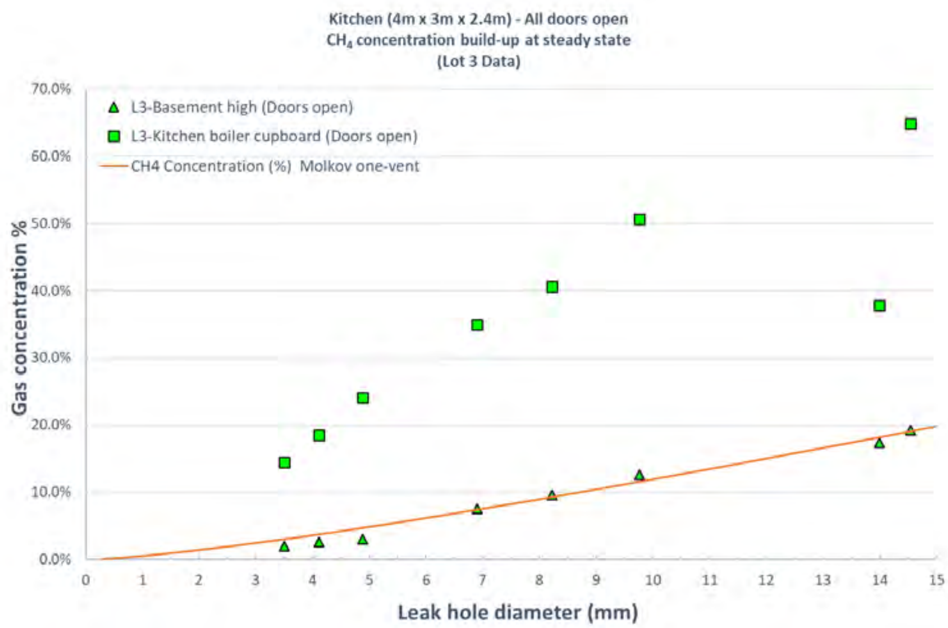

Figure 21: Comparison of predicted and measured peak CH_4 concentrations in kitchen resulting from basement and kitchen boiler cupboard releases (all doors open, assumed total leak and vent area = $0.2m^2$)

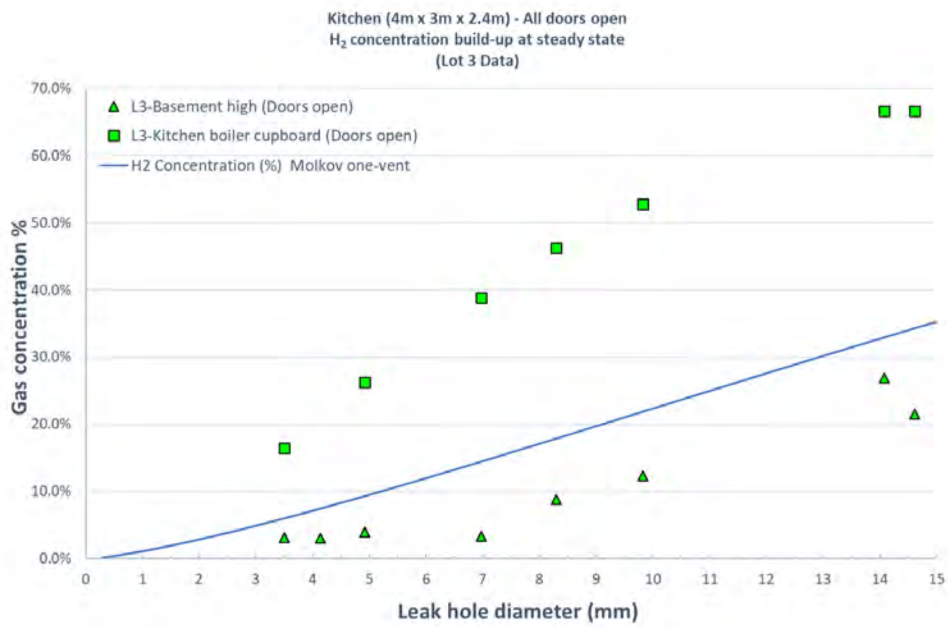

Figure 22: Comparison of predicted and measured peak H_2 concentrations in kitchen resulting from basement and kitchen boiler cupboard releases (all doors open, assumed total leak and vent area = $0.2m^2$)

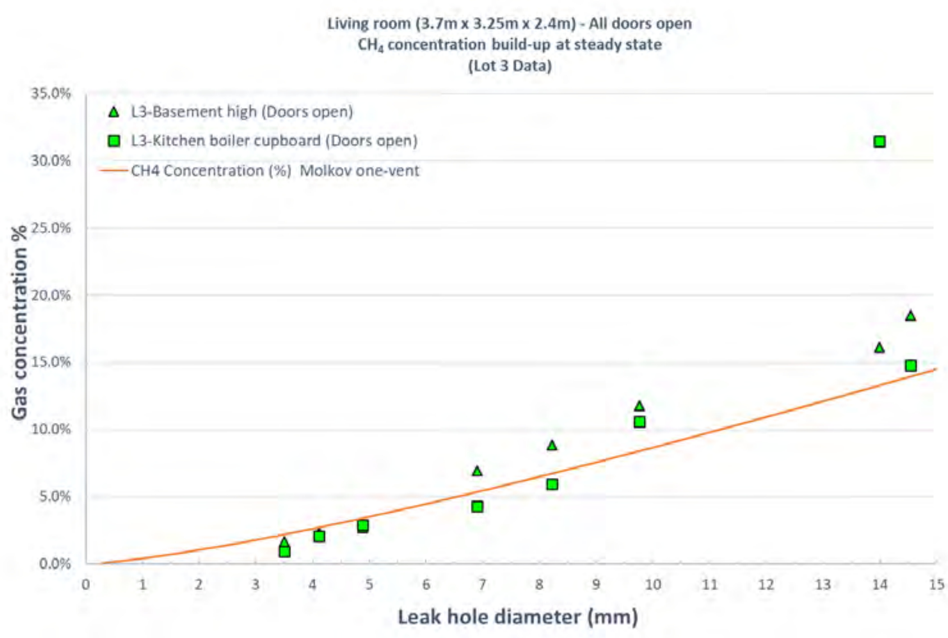

Figure 23: Comparison of predicted and measured peak CH_4 concentrations in living room resulting from basement and kitchen boiler cupboard releases (doors open, assumed total leak and vent area = $0.30m^2$)

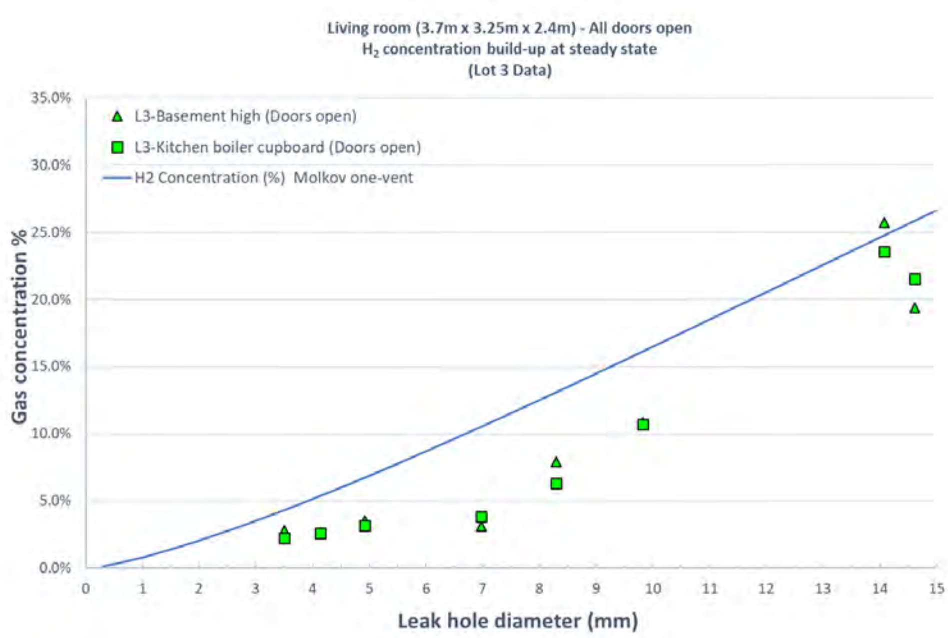

Figure 24: Comparison of predicted and measured peak H_2 concentrations in living room resulting from basement and kitchen boiler cupboard releases (doors open, assumed total leak and vent area = $0.30m^2$)

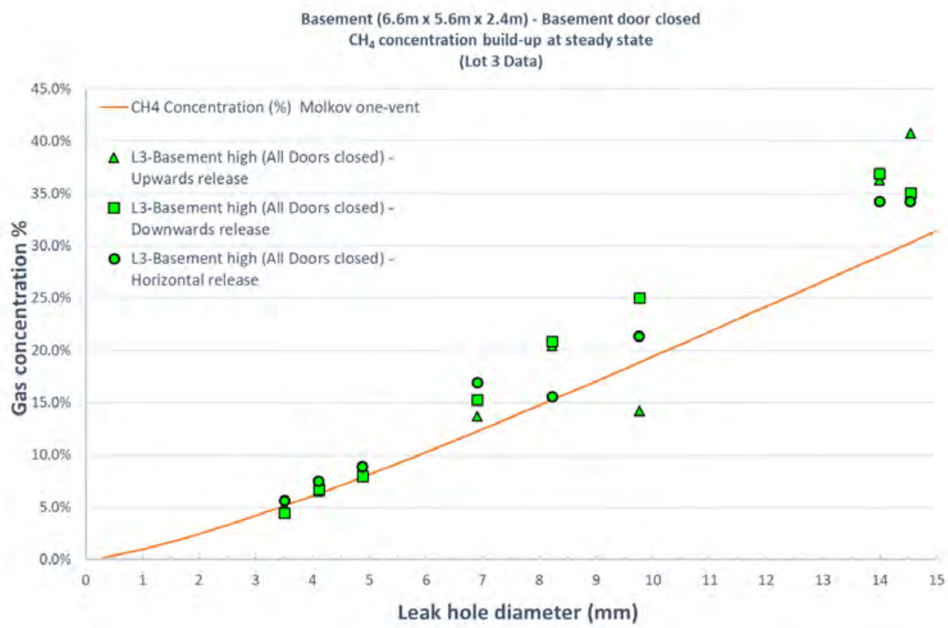

Figure 25: Comparison of predicted and measured peak CH_4 concentrations in basement resulting from basement releases (basement door closed, assumed total leak and vent area = $0.11m^2$)

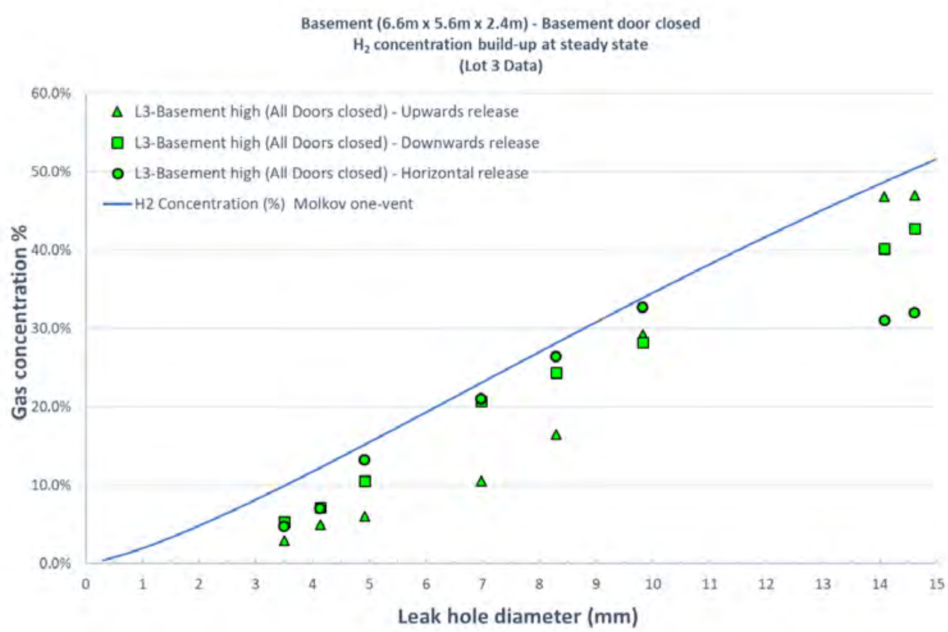

Figure 26: Comparison of predicted and measured peak H_2 concentrations in basement resulting from basement releases (basement door closed, assumed total leak and vent area = $0.11m^2$)

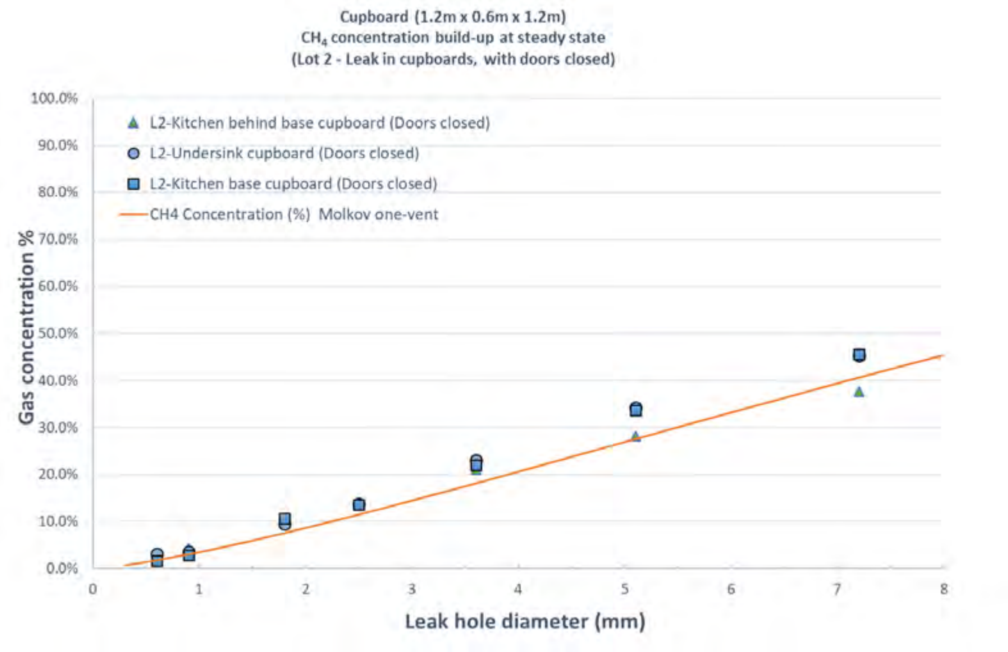

Figure 27: Comparison of predicted and measured peak CH_4 concentrations in cupboard (cupboard door closed, assumed total leak and vent area = $0.02m^2$)

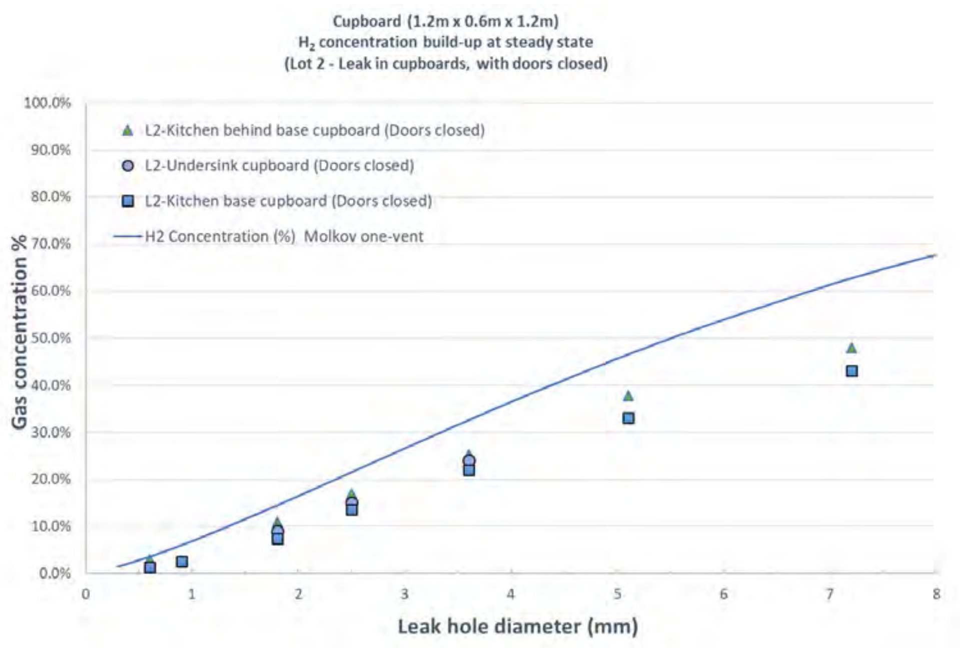

Figure 28: Comparison of predicted and measured peak H_2 concentrations in cupboard (cupboard door closed, assumed total leak and vent area = $0.02m^2$)

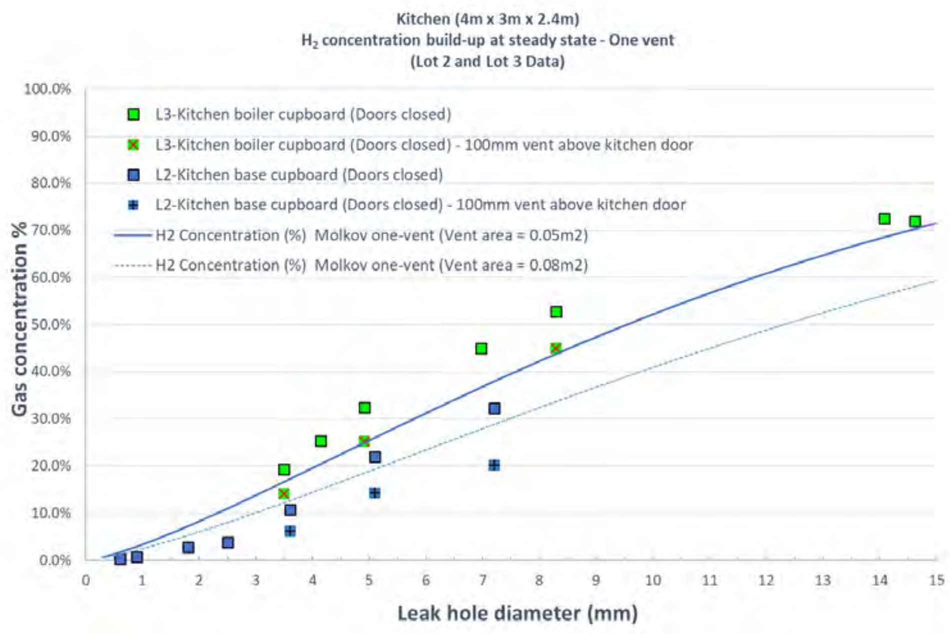

Figure 29: Comparison of predicted and measured peak H_2 concentrations in kitchen (∅ 100mm vent hole above the kitchen door, assumed total leak and vent area of $0.05m^2$ and $0.08m^2$)

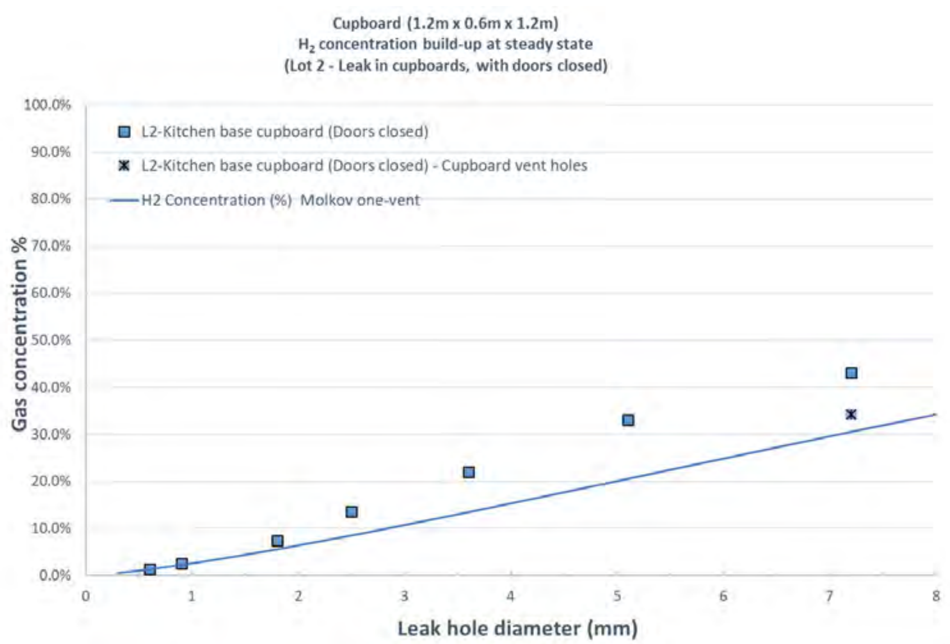

Figure 30: Comparison of predicted and measured peak H_2 concentrations in cupboard (8x ∅ 100mm vent holes in the cupboard, assumed total leak and vent area = $0.08m^2$)

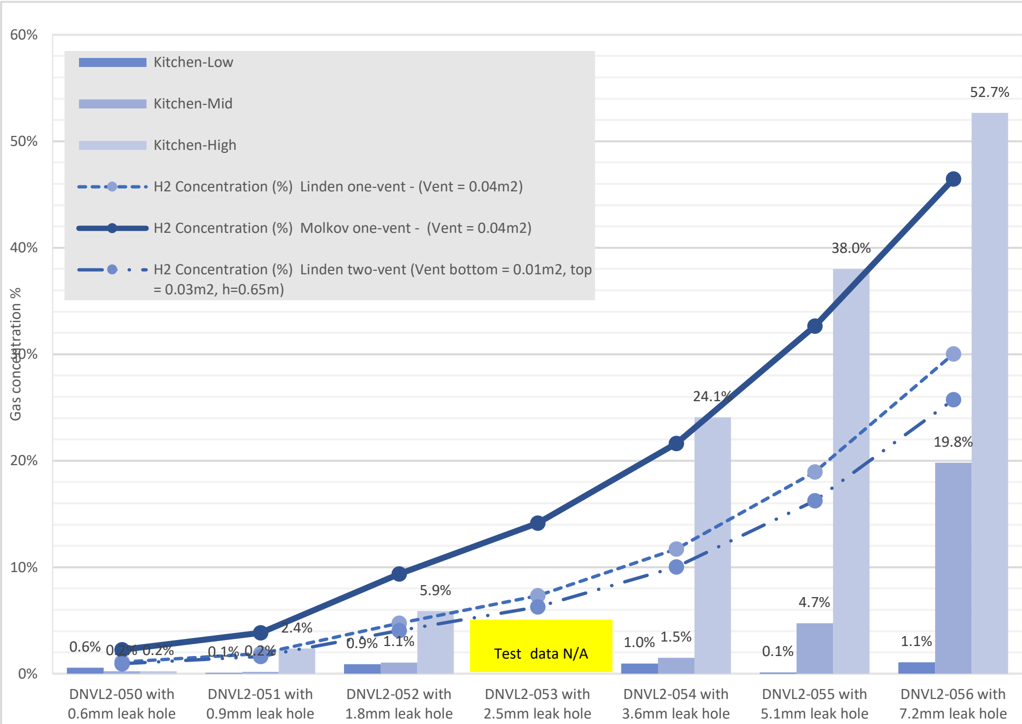

Figure 31: Dispersion model results for peak H2 concentration build-up in comparison with Lot 2 DNV Tests L2-050 to L2-056 (Leak in kitchen wall cupboard, with doors closed)

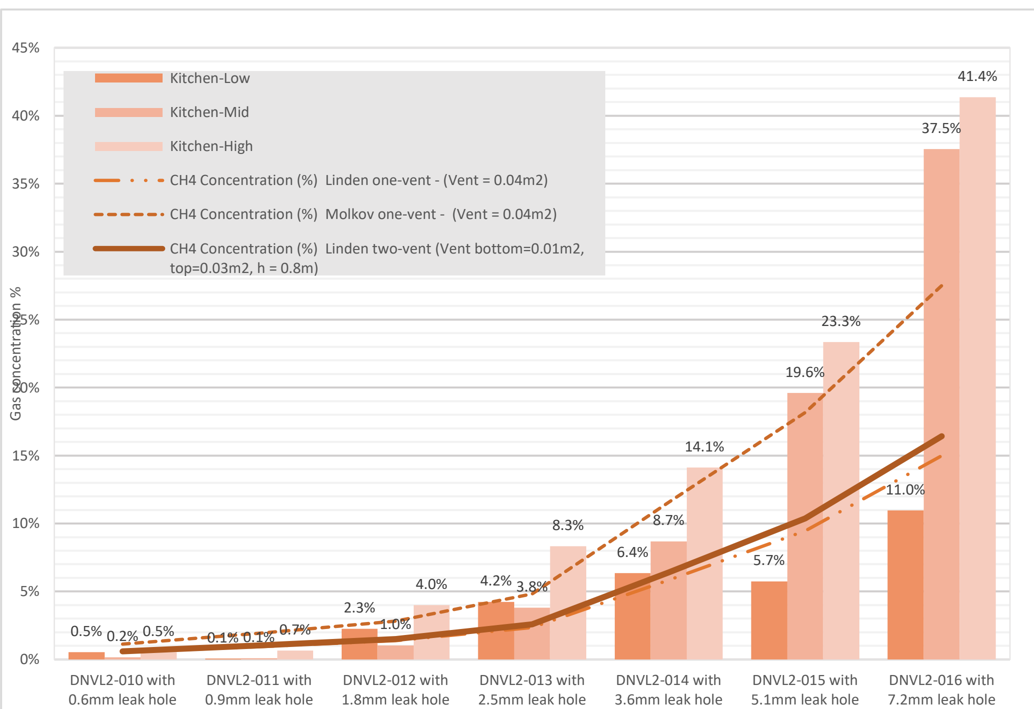

Figure 32: Dispersion model results for peak CH_4 concentration build-up in comparison with Lot 2 DNV Tests L2-010 to L2-016 (Leak in kitchen wall cupboard, with doors closed)

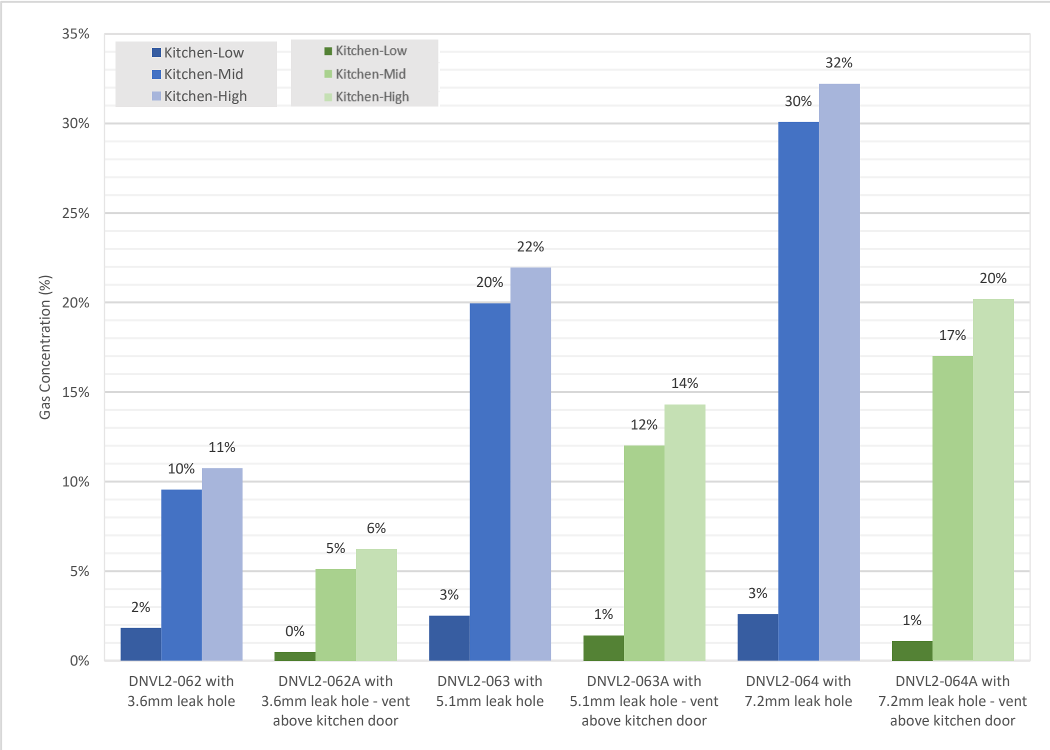

Figure 33: Comparison of experiment results for peak H_2 concentration build-up resulting from leak in kitchen base cupboard, with a 100mm diameter circular vent added above the kitchen door (green bars) and no-vent cases (blue bars)

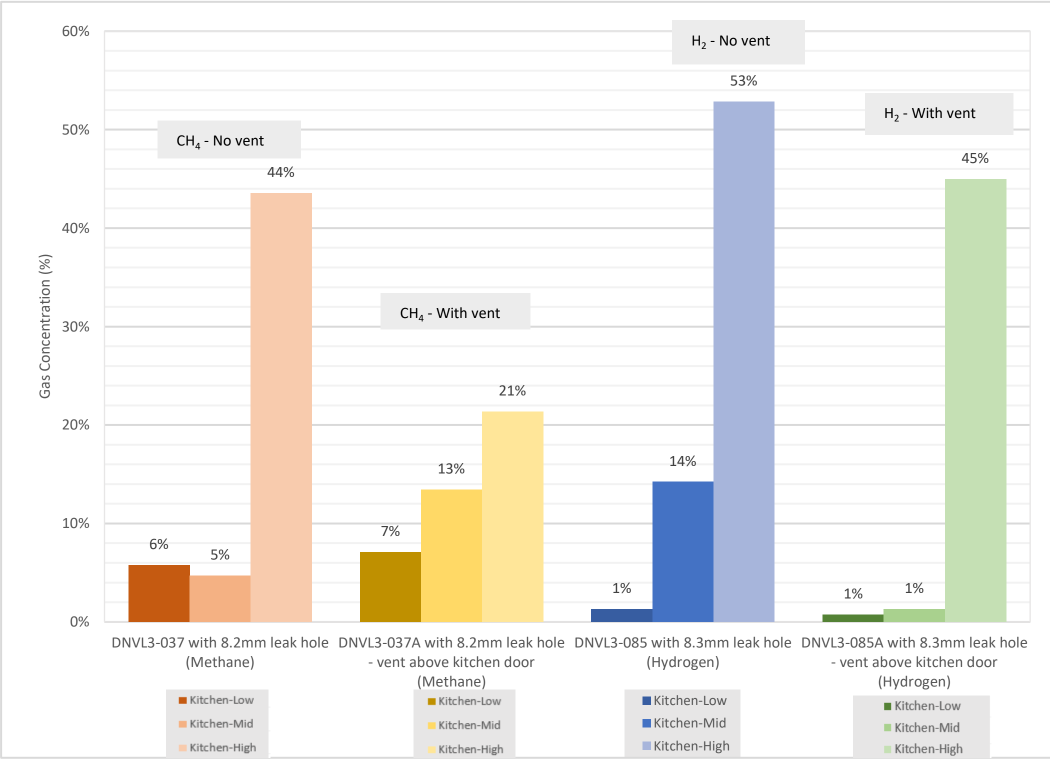

Figure 34: Comparison of experiment results for peak CH_4 and H_2 concentration build-up resulting from leak in kitchen boiler cupboard, with a 100mm diameter circular vent added above the kitchen door

6. Dispersion model charts for the QRA framework

Based on the observations from the WP7 experimental data for the air permeability rates and concentration data for hydrogen and methane, the following spaces are considered to be included in the QRA framework to represent spaces within a typical domestic house (Table 1) considering the dimensions of the spaces used for WP7 test programme:

Table 9: Gas leak locations and representative air tightness levels

Gas leak locations:	**Cupboard**		**Kitchen**		**Storey (Downstairs of a terraced house)**	
Space dimensions (width x length x height)	1.2m x 0.6m x 1.2m		4m x 3m x 2.4m		8m x 4m x 2.4m	
Volume size (in approximation with potential leak locations)	~1 m^3		~ 30 m^3		~75 m^3	
Air leakage & vent assumptions (For the definition of leakage and vent please refer to Section 3.2)	**Total leak & vent area**	**Air permeability rate estimated @50Pa**	**Total leak & vent area**	**Air permeability rate estimated @50Pa**	**Total leak & vent area**	**Air permeability rate estimated @50Pa**
Highly sealed (e.g. no added ventilation)	~ 0.02 m^2	8 $m^3/(h.m^2)$	~ 0.04 m^2	2 $m^3/(h.m^2)$	~ 0.04 m^2	1 $m^3/(h.m^2)$
Moderately sealed (e.g. added ventilation through vent area above door or old house conditions with leak through cracks)	~ 0.03 m^2	15 $m^3/(h.m^2)$	~ 0.08 m^2	5 $m^3/(h.m^2)$	~ 0.15 m^2	5 $m^3/(h.m^2)$
Leaky (e.g. more added ventilation provided by continuous vent above doors and /or open door)	~ 0.05 m^2	25 $m^3/(h.m^2)$	~ 0.20 m^2	15 $m^3/(h.m^2)$	~ 0.40 m^2	15 $m^3/(h.m^2)$

The levels of air permeability rate chosen in Table 9 are roughly aligned to a study published by Leeds Metropolitan University which analysed data from BRE's database of air leakage. This data contained information on 471 properties of different age size, type and construction [28] and showed that a very wide range of air permeability rate exists within the UK housing stock, with 37% of the housing stock having air permeability rate between 5 $m^3/(h.m^2)$ - 10 $m^3/(h.m^2)$ and 59% of the dwellings having air permeability rate more than 10 $m^3/(h.m^2)$. 4% of properties have permeabilities below 5 $m^3/(h.m^2)$.

Unfortunately, it has not proved possible to find published data on the permeability of individual rooms such as kitchens, bathrooms and utility spaces where boilers are commonly installed, although these often require (by law) a minimum of ventilation to control damp.

The DNV GL experiments carried out as a part of Hy4Heat provide a means to judge (in a preliminary way) what might be considered normal – at least for a kitchen. The DNV GL kitchen has leaks at various levels due to cracks in the floor, drains and other plumbing, incomplete floor seal, electrical fittings e.g. sockets and lights etc. In all these respects it could reasonably be considered typical. The DNV GL trial building was a new setup which can be considered with a reduced the level of leakage but has a sub-floor which might increase the leakage level.

The DNV GL kitchen does however differ from properties that comply with Building Regulations Approved Document F (AD(F)) [29], in that it does not have a means of continuous ventilation. Therefore, it is assumed in the QRA [12] that the level of background leakage of properties in the “Highly sealed” category (less than 5 $m^3/(h.m^2)$ – frequency 4%) correspond to those in the DNV GL house without continuous kitchen ventilation. The value of 0.04 m^2 total vent area produced dispersion model predictions that fit well with the WP7 DNV GL test data without any added ventilation above kitchen door (Section 5.3).

The moderately sealed category is assumed to correspond to kitchens that have similar background leakage to the DNV GL kitchen but have additional ventilation to satisfy AD(F) – which should be continuously available. This assumption is based on the dispersion model results with the value of 0.08 m^2 total vent area producing acceptable predictions of DNV GL experiments carried out with the additional 100mm diameter vent hole above the kitchen door (Figure 29).

This means that the results in the QRA are applicable to a population of properties (e.g. in a trial) where steps have been taken to ensure compliance with AD(F) [29] in a suitable manner.

Assumed airtightness properties and enclosed space sizes listed in Table 9 will be updated as necessary depending on the selected event trees for the QRA, and appropriate gas concentration curve will be developed for each enclosed space considering the defined vent properties, e.g. doors closed / open, vent over the doors, etc. Therefore, subsequent sections include representative dispersion model data obtained with one-vent Linden model which will be integrated to the QRA framework for the consequence assessment.

6.1 Cupboard (1.2m x 0.6m x 1.2m)

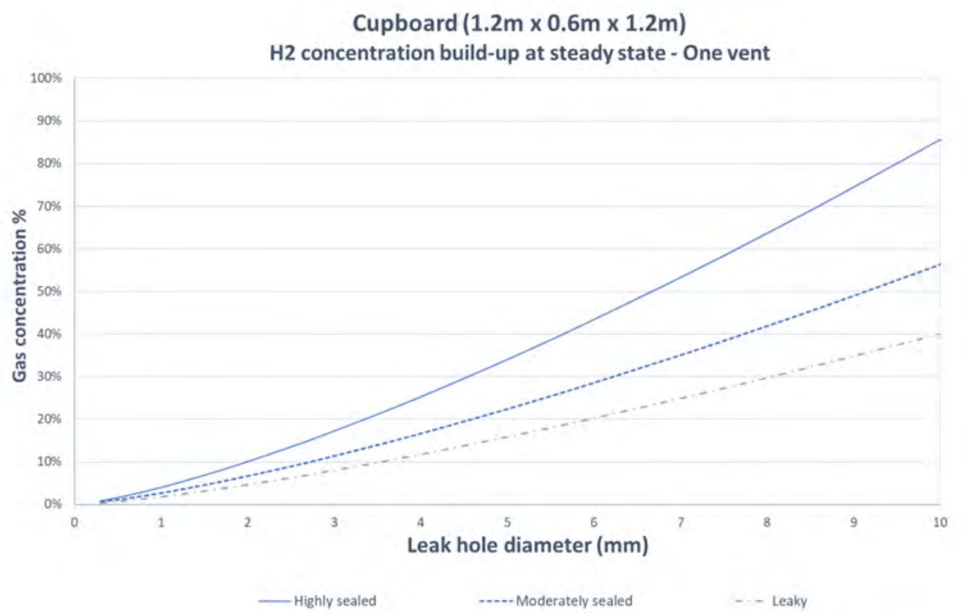

Figure 35: Representative QRA Input: Peak H_2 concentrations in cupboard for three different levels of air tightness: highly sealed, moderately sealed, and leaky

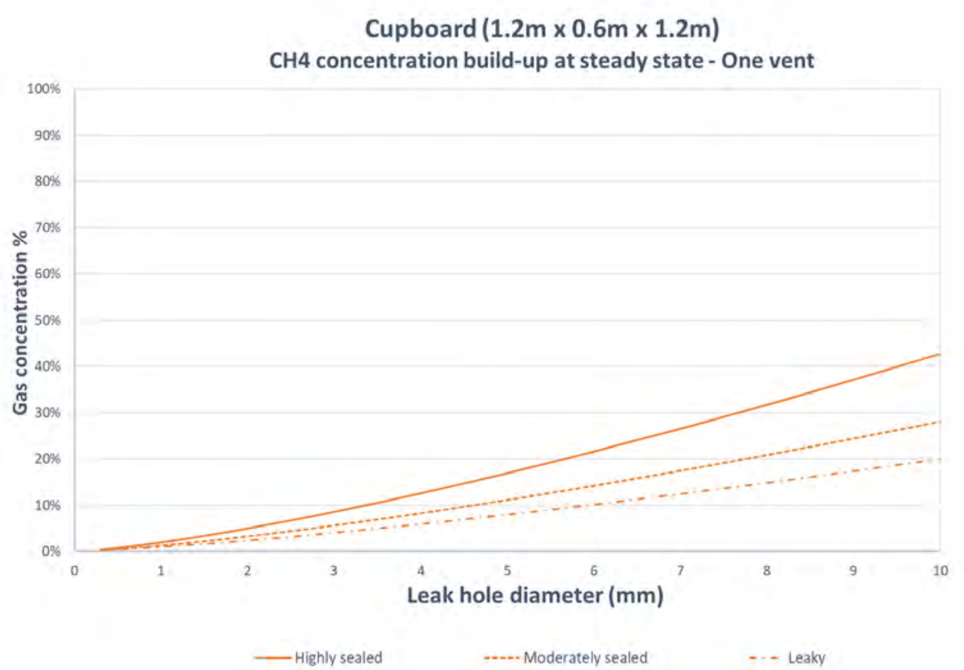

Figure 36: Representative QRA Input: Peak CH_4 concentrations in cupboard for three different levels of air tightness: highly sealed, moderately sealed, and leaky

6.2 Kitchen (4m x 3m x 2.4m)

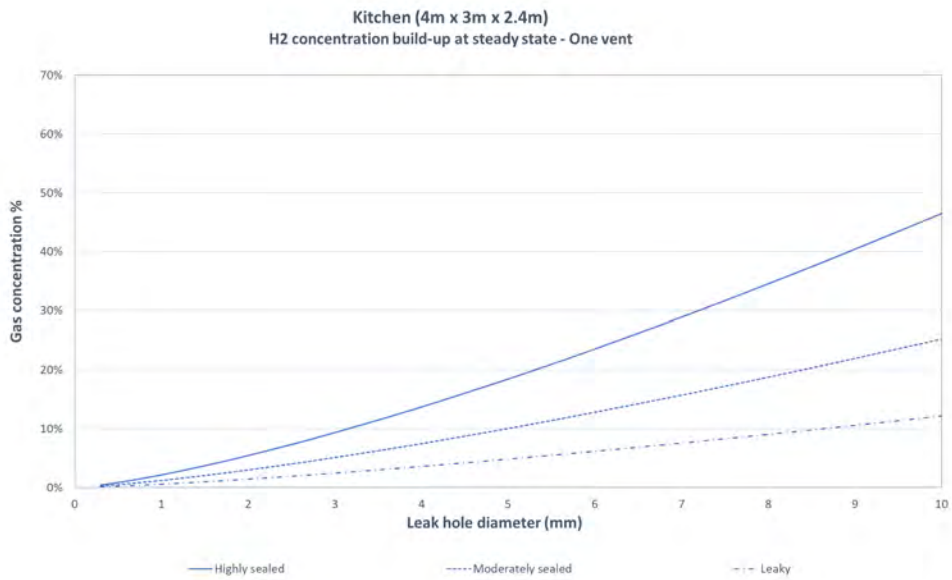

Figure 37: Representative QRA Input: Peak H_2 concentrations in kitchen for three different levels of air tightness: highly sealed, moderately sealed, and leaky

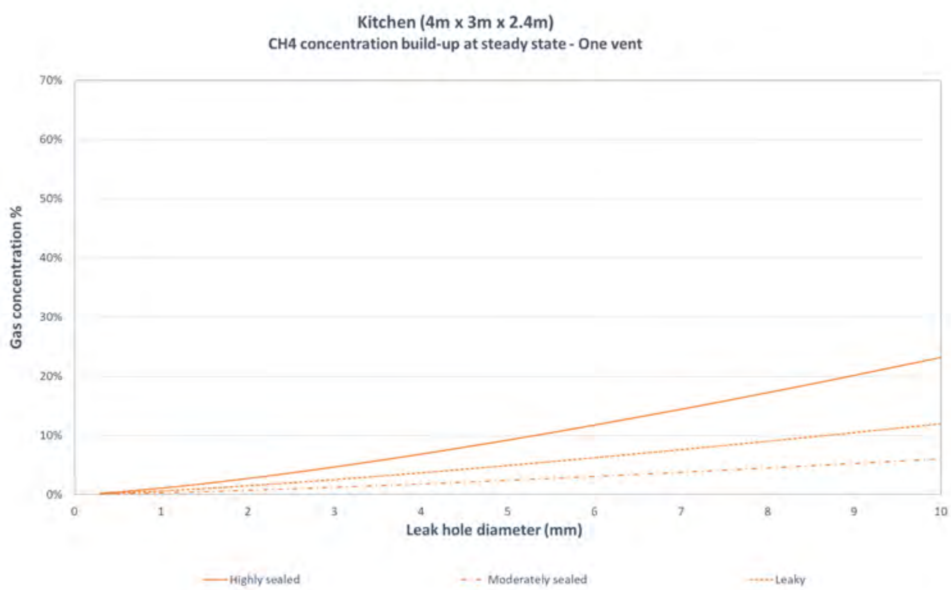

Figure 38: Representative QRA Input: Peak CH_4 concentrations in kitchen for three different levels of air tightness: highly sealed, moderately sealed, and leaky

6.3 Storey (Downstairs of a terraced house) (8m x 4m x 2.4m)

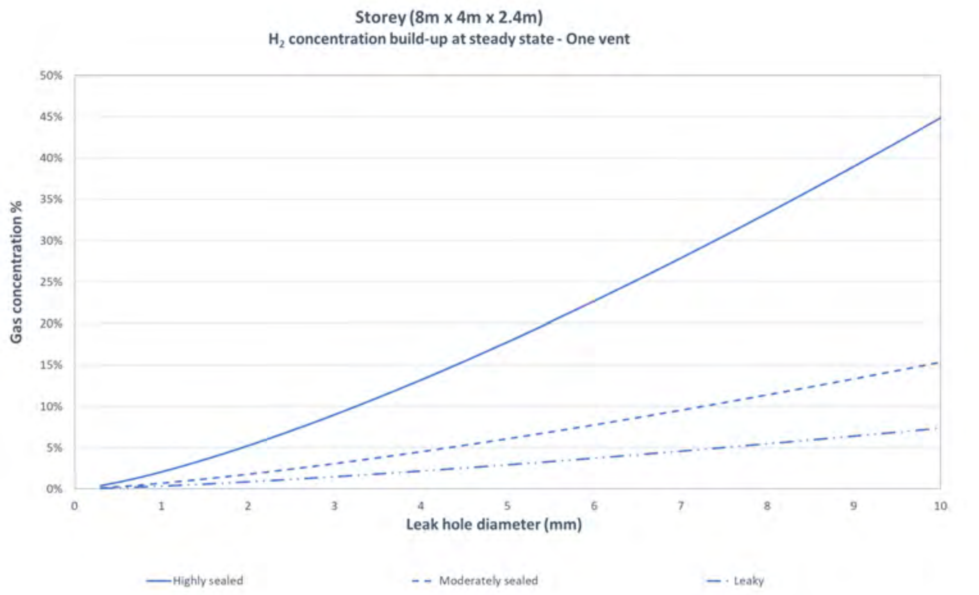

Figure 39: Representative QRA Input: Peak H_2 concentrations in storey for three different levels of air tightness: highly sealed, moderately sealed, and leaky

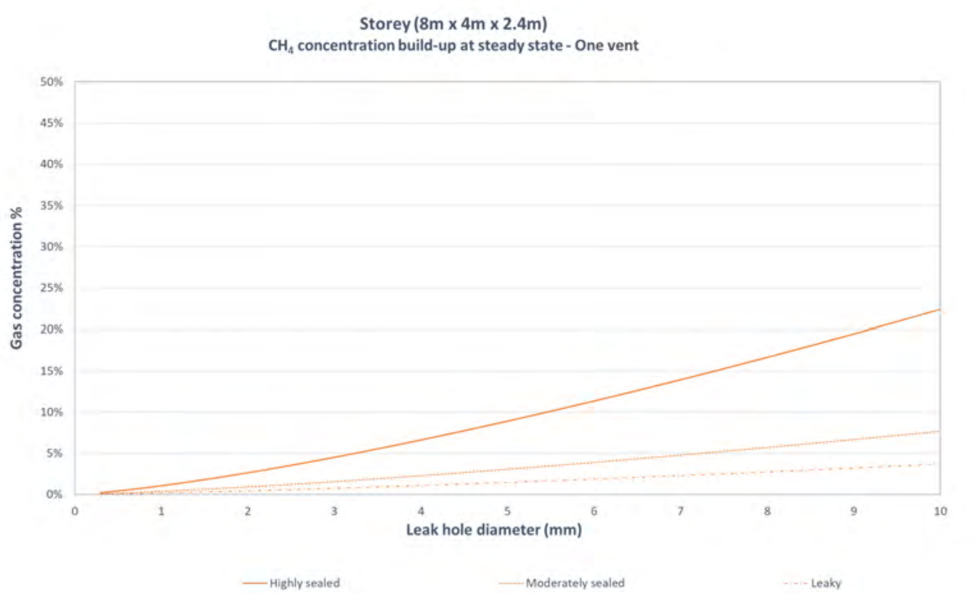

Figure 40: Representative QRA Input: Peak CH_4 concentrations in storey for three different levels of air tightness: highly sealed, moderately sealed, and leaky

7. Conclusions and recommendations for further work

Identification and validation of simplified dispersion models for hydrogen (H_2) and methane (CH_4) have been addressed in this report. As a result, accurate, simple, rapid and validated dispersion models, namely Linden model or Molkov model, are used to develop the dispersion modelling part of the QRA. Nevertheless, there still exist gaps which need to be filled at this point. These are summarised as follows:

- As noted above, the theoretical results underestimate experimental results for the leak scenarios where the leaks were located at high levels of the floor. This is due to the fact that the estimation of hydrogen concentration was limited to the capability of the modelling. It is therefore suggested that experimental results are directly used in the QRA or the conservative results from the dispersion model are used for the steady-state concentration of hydrogen.
- WP7 DNV tests did not provide detailed data on the air permeability rate of individual rooms which depends on the properties of the natural ventilation, openings and ducts and the amount of leak through the building structure. Therefore, test data for different rooms under different test configurations (e.g. doors open vs. doors closed) are estimated using the available Lot 2 and Lot 3 test data. Additional investigation on the effect of wind and natural ventilation parameters (e.g. air permeability rate or air change per hour, *ACH*; size, location and number of vents; winds etc. at each enclosed space) on dispersion of hydrogen should be performed for more accurate dispersion model predictions.

8. References

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