International Journal of Hydrogen Energy 56 (2024) 797–806

Contents lists available at ScienceDirect

International Journal of Hydrogen Energy

journal homepage: www.elsevier.com/locate/he

Numerical modelling of hydrogen leakages in confined spaces for domestic applications

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A R T I C L E I N F O

Handling Editor: Dr J Lobato

Keywords:
Hydrogen
Energy
Security
Modelling and simulation
Gas leak

A B S T R A C T

The UK government tentatively plans to use hydrogen for domestic applications by 2035. While the use of hydrogen aims to reduce the dependence on hydrocarbons, certain factors need consideration. Since hydrogen is much lighter, and more reactive than methane, it is crucial to understand the change in risk for accident scenarios involving hydrogen in a domestic setting. Numerical modelling was used to simulate the leakage of hydrogen and methane in small, enclosed spaces such as kitchen cupboards. The k- ε turbulence model was used along with the species transport model to simulate the leakage of gas for different inlet locations and leak diameters (1.8 mm–7.2 mm). From the modelling study, it was observed that hydrogen and methane both tend to stratify from top of the control volume to the bottom. The key finding was that, under adverse conditions (leak from a 7.2 mm diameter hole) and due to greater volumetric flow, hydrogen tends to reach equilibrium concentration 45s faster than methane for a total leak duration of 600s. Additionally, it was noted that cases with leak inlet locations near corners had 28% lower hydrogen concentrations, and 25% lower methane concentrations as compared to leak inlet locations near the centre of the cupboard.

1. Introduction

The UK government tentatively plans to use hydrogen for domestic applications by the mid-2030s as part of its hydrogen strategy [1]. The use of hydrogen is intended as a method to phase out the use of hydrocarbon fuels such as methane (key component of natural gas), thus reducing greenhouse gas emissions [2–4]. Hydrogen is being considered as a fuel for this application due to its reaction products (water) having a negligible global warming potential (0.005) [5]. Methane's reaction products (Carbon dioxide and water) have a higher global warming potential ($GWP_{CO2} = 1$; $GWP_{water} = 0.0005$) [5]. To bolster the push towards Hydrogen, the UK government (and other governments around the world) are actively creating policies to financially support the production and use of hydrogen; and create a safety case for its consumption [6–13]. While the use of hydrogen as a fuel is not a new idea, the production of hydrogen is expensive, and requires government support to encourage stakeholders to invest in it [10,14–16]. The investment from various stakeholders in the production of Hydrogen would be a step towards reducing the cost of the fuel, thus making it attractive to the consumer [10,17].

While government policy is favouring hydrogen as an energy vector, it is important to understand and ensure the safety of the fuel during consumption. The three key concerns with respect to hydrogen are its extremely low ignition energy (0.019 mJ); wide flammability range in air (4–75%); and its fast laminar burning velocity (3.20 m/s) [18–21]. Methane on the other hand has a higher ignition energy (0.300 mJ); a limited flammability range (5–15%); and slower laminar burning velocity (0.25 m/s) [21–23]. In addition to this, methane and hydrogen have very different physical properties (Table 1), which in turn increases the need for a safety case when shifting from methane to hydrogen [21,24].

The difference in density, viscosity, and mass are suggestive of a difference in the way the gases must be handled, especially during transport and combustion [25,26]. Additionally, the creation of a safety case in conjunction with an understanding of the gas' properties can be used to provide guidance to the consumer when they use the fuel. Given the differences in ignition energy, flammability range, and laminar burning velocity, it is important to note the difference in reactivity of hydrogen and methane. The reactive nature of hydrogen poses a higher threat of detonation in accident scenarios as well. Having established the inherent differences in the properties of methane and hydrogen, it is important to understand its threat profile. Here threat profile is used to

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https://doi.org/10.1016/j.ijhydene.2023.12.279
Received 5 October 2023; Received in revised form 8 December 2023; Accepted 26 December 2023
Available online 1 January 2024

refer to the risk of deflagration or detonation with respect to hydrogen leakage. For the purpose of this study, leakage refers to the flow of gas from a pipe through a hole of fixed diameter [27,28].

1.1. Literature Survey

Due to the focus on hydrogen as an energy vector for the future, it has actively been used in the industry as a thermally efficient fuel, in conjunction with methane [29–31]. The key risks associated with hydrogen are that of leakage, and the consequent fire and explosion (due to its low ignition energy) [24]. The leakage of hydrogen (or hydrogen/methane) has been studied for various cases pertaining to the transport and storage of hydrogen [32–35]. The work by Liu et al. (2018) [34], looked at high pressure leakages (when the gas is stored at pressures up to 90 MPa) of hydrogen and the simulation of jet fires because of these leakages. This work sheds light on the risk of gas leaks from pipelines in an open space and the prediction of jet fires in the process. While modelling was used for the prediction of the jet fire, little description was provided regarding the diffusion of the gas, and its influence on the jet fire formation.

Another aspect of hydrogen leakage in open spaces was studied by Liang et al. (2019) [32], in their modelling of hydrogen leakage and explosion at a refuelling station. This work focused on the influence of external factors such as wind direction, leakage direction, and the presence of obstacles on the prediction of risk and the severity of the consequence. The key findings of this research allowed for an empirical understanding of the threat profile of hydrogen. While useful, the results of this study were focused to a very specific case, thus limiting their overall value.

Focusing on the theme of leakages in open spaces, the study by Chen and Mao (2017) [35] looked at the use of modelling for the prediction of the size of the vapour cloud when hydrogen leaked from a pipeline. This simulation study looked at the influence of ambient conditions (wind speed, temperature, and humidity) on the hydrogen diffusion, and the effect of this on the consequences of the leak (sustained combustion or vapour cloud explosion). While this study is based on a singular incident, it highlights key factors that must be considered when simulating gas leaks.

While open air leakages are more likely for certain hydrogen fuel applications, it is also vital to consider the risks of hydrogen leaks in confined spaces [33,36,37]. The leakage of hydrogen in a confined space has a higher risk of combustion or detonation due to the accumulation of the gas [37]. As a result of this, factors such as the presence of obstacles; presence of vents; gas turbulence; and gas concentration influence the threat profile of hydrogen [38–48]. The work done by Li et al. (2023) focused on the simulation of hydrogen blended natural gas leakages in a domestic setting [49]. Compared to conventional approaches for simulating gas mixing, this study did not use species transport equations and focused on the turbulence modelling. This study highlighted the importance of ventilation in a gas leak scenario, and how it is a key factor to consider when assessing the risks of hydrogen blended natural gas. Subsequently, the influence obstacles on hydrogen diffusion in confined spaces was carried out by Kang et al. (2024) [50]. This study looked at the interaction of hydrogen with a regularly shaped obstacle and how that influenced the efficiency of diffusion, kinetic energy of the gas, and the consequent risk of accidental initiation. The research on the risk of hydrogen has been focused on large scale applications such as industry, and national transport infrastructures, with little focus on the potential for hydrogen consumption at the domestic level. While the interest in hydrogen as a domestic fuel has been growing, little work has been done to identify its threat profile at that scale [27,28].

For the domestic setup, the same factors would influence the combustion and detonation risk of hydrogen in a confined space, but there would be differences in terms of the geometry and structure of the domain. Compared to industrial setups or large transport systems, the venting in a domestic setting would be different, and the type of obstacles in the space would be different as well. Consequently, the application of findings from existing modelling studies on hydrogen leakage and combustion are less likely to be applicable for the domestic case. This results in the need for further study regarding the leakage of hydrogen in a domestic setting, and the subsequent threat it poses.

1.2. Objective

Based on the literature review, it was noted that a large section of the work was focused on the process of combustion, and detonation of hydrogen. Furthermore, research in the wider literature looked to study the detonation of hydrogen-methane blends, because that is the fuel being widely used in industrial applications. As a result, the context of the literature is centred around industrial cases, and the explosion risk pertaining to them. With previous studies focusing on the detonation of hydrogen (or hydrogen-methane blends) in confined space, only a few studies have been done to visualise the diffusion and leakage of gas. Additionally, findings from modelling and experimental work designed for industrial cases may not be directly translatable to the domestic environment.

Consequently, the key objective of this study is to use numerical modelling to identify key differences between hydrogen and methane during leakage scenarios in small, confined spaces (i.e., a wall cupboard in a kitchen). The leakage of the two gases will be compared based on their concentration in air. The study will look at the influence of inlet diameter and inlet location on the diffusion of gas within the space. Methane was selected as it is a major component of natural gas, and it would allow for better replicability of the study while reducing the error caused by variation in the trace components in natural gas. The variation of inlet diameter (1.8 mm–7.2 mm) simulates different sizes of leaks, and the inlet location simulates the various locations at which the gas distribution pipe enters the cupboard.

2. Methodology

This study used numerical modelling to understand the process of gas accumulation in small, confined spaces. The leakage process of methane (as a representative of natural gas) and hydrogen were compared for varying inlet diameters (1.8 mm–7.2 mm) and inlet locations along a single face of the problem domain. The inlet diameters, inlet flow parameters, and locations were selected to allow for the modelling study to be validated against previous experimental work done in the Hy4Heat project [28].

2.1. Model setup

Computational fluid dynamics software (ANSYS Fluent 2020R2) was used to simulate the turbulent flow and diffusion of gas within a kitchen cupboard. Fig. 1 shows the simulation setup. The cupboard dimensions (770 mm × 760 mm x 355 mm) were selected based on an average kitchen cupboard available from a large retailer and to allow comparison with previous experimental work [28]. The run time for the

Table 1
Chemical properties of Methane and Hydrogen.

Gas	Density (kg/m^3)	Viscosity (Pa.s)	Ignition energy (mJ)	Flammability Range (% in air)	Energy Density (MJ/kg)	Laminar Burning Velocity (m/s)
Hydrogen	0.0832	8.760×10^{-6}	0.019	4–75	120	3.20
Methane	0.6640	1.084×10^{-5}	0.300	5–15	50–55	0.25

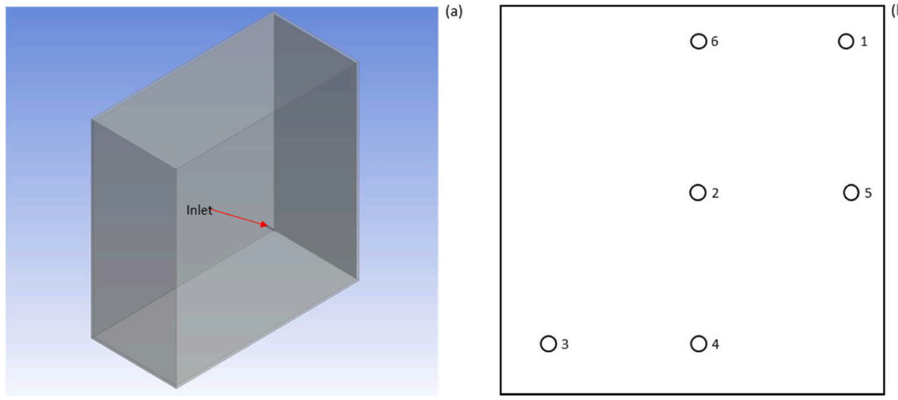

Fig. 1. Visualisation of cupboard geometry using (a) isometric view of the cupboard; and (b) Location of different gas inlets on the back face of the cupboard.

simulation was 600s as the control volume being considered is relatively small compared to the inlet parameters of the gas. Therefore, a simulation of 600s would be able to highlight the gas movement within the problem domain (i.e., the wall cupboard). The key assumptions made in the model were (i) there was no venting in the cupboard; (ii) the gas mixtures (methane-air; hydrogen-air) do not react; and (iii) there is no temperature change during the diffusion process.

The k-ε model for turbulent flow was used in conjunction with the species transport model for inlet diffusion to simulate the leakage of gas into the fluid domain of the cupboard geometry. The k-ε model was chosen because it is more reliable for fluid flow in confined space and accounts for diffusive transport [51]. The species transport model was chosen to simulate the diffusion of incoming gas within the fluid domain of the cupboard. The species transport model was chosen because it is widely used for the simulation of gas mixing in confined spaces, especially for reactive gases [43,52–54]. While this model is usually considered for the simulation of combustion reactions, it is also viable for predicting the mixture of gases and their movement, at a molecular level, within a domain [53,54]. Table 2 shows the inlet parameters for the modelling study. These conditions were selected to simulate the experiments carried out by Simpson et al. (2019) [28]. The inlet diameter refers to the diameter of the location through which the leakage process is being simulated. Additionally, the different velocities of hydrogen and methane are representative of similar pressure loss (per unit distance) conditions during adverse transport conditions [24]. The geometry was kept constant for all cases, and the size of the leak was changed by altering the hydraulic diameter boundary condition. This was done by changing the corresponding inlet parameters for hydraulic diameter and turbulence intensity (used to represent the Reynolds number), to represent the various leak diameters.

Table 2
Inlet boundary conditions for the simulation of Methane and Hydrogen leak in a confined space.

Gas	Inlet Diameter (m)	Volumetric flowrate (m^3/h)	Velocity (m/s)
Methane	18e-4	0.40	43.66
Methane	25e-4	0.80	45.27
Methane	36e-4	1.60	43.66
Methane	51e-4	3.20	43.51
Methane	72e-4	6.40	43.66
Hydrogen	18e-4	1.15	125.53
Hydrogen	25e-4	2.20	124.49
Hydrogen	36e-4	4.59	125.26
Hydrogen	51e-4	9.21	125.24
Hydrogen	72e-4	18.36	125.26

2.2. Meshing

A fidelity study was conducted on the computer (Lenovo Thinkstation; Intel i9 processor 3.10 GHz; 64 GB RAM) used for the simulations to understand the effect of the cell size used in the problem domain on the accuracy and computation time of the simulation. The fidelity study was carried out for a 7.2 mm leak for hydrogen. While the main simulations were looking at leak scenarios for 600s, this computational model was run for a shorter time (300s instead of 600s) for the problem domain (770 mm × 760 mm x 355 mm) to carry out the fidelity study and ensure mesh independence. Table 3 shows the findings from the meshing study.

For the residue condition of 10^{-4}, the simulation converged for all three mesh cases. From Table 3, the solutions (H_2 mole fraction in air) of the computational model were within 2% of each other for different mesh sizes, thus suggesting mesh independence. Based on that, a mesh size of 2.75×10^{-2}m was selected for the simulations as it had the highest fidelity. Subsequently, the other models were meshed with a similar number of nodes to allow for better comparison of the results. Fig. 2 shows a representative mesh of the fluid domain within the control volume. The mesh has been given a growth factor to allow for high fidelity at the inlet, and lower fidelity closer to the edges. This allows for accurately measuring the flow of gas during the initial seconds of the process without compromising on findings during the remainder of the simulation.

2.3. Post processing and data collection

The solutions from the simulations were post processed on Paraview v5.11 (open-source code) and the mole fractions of hydrogen and methane during leakage scenarios were measured [55]. Initially, the measurement of gas concentration was carried out by placing a probe at the furthest point from the inlet location. This was done as it would represent the worst-case scenario of the gas diffusion within the domain. An error with this approach was that it did not account for the dynamic movement of the gas and produced data that had errors. Since the k-ε model used in the study did not use enhanced wall interaction models, placing the probe near the edge of the box created a source for errors. Furthermore, the probe location was close to the walls of the box, which could allow the turbulent gas interactions with the wall to influence the

Table 3
Key findings from fidelity study for the simulation of hydrogen gas leaks in a closed cupboard.

Element size (m)	Number of Nodes	Run Time (s)	H_2 mole fraction in air
2.75×10^{-2}	33540	258	0.198
3.00×10^{-2}	31059	323	0.201
3.25×10^{-2}	29258	215	0.205

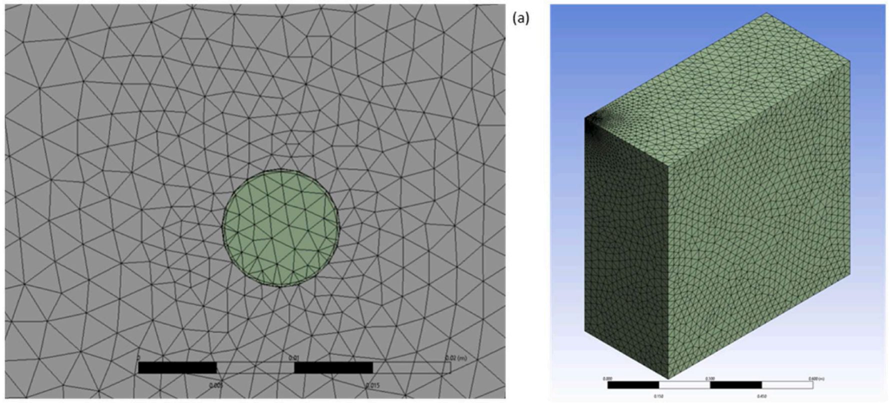

Fig. 2. Representative mesh for (a) Gas inlet (green); and (b) graded mesh for fluid domain to allow for visualisation of gas leak. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

concentration measurement.

To therefore improve the reliability of the results, an array of probes at fixed locations was used to measure the gas concentrations, and an arithmetic mean of those measurements was used as the gas concentration at a given point of time. Based on existing literature, it was known that hydrogen and methane, being lighter than air, tend to stratify [28,35]. In this case, the use of the term stratify refers to the tendency of the gas to rise upwards due to it being lighter than air. This implies that the gas is more likely to accumulate towards the top of the domain. Consequently, the array of probes was located near the top of the box with adequate distance (57.5 mm) from the walls to minimize the influence of wall interactions (Fig. 3).

3. Results and discussion

3.1. Comparison of gas leakage behaviour

Hydrogen and methane are both light gases and are less dense than air [28,35]. The low density implies the tendency of both gases to move upwards and stratify in air. Additionally, their relatively low viscosities allow for minimal resistance during turbulent flow conditions. The leakage process for hydrogen and methane within the cupboard is shown in Figs. 4 and 5, respectively. Each figure shows the cross-section of the domain at different time steps to visualise the transport of gas from the inlet. In this case, the differing inlet conditions also influenced the movement of gas within the fluid domain. In addition to these factors, the physical properties of the molecules also affect the transport of gas within the system e.g. density and viscosity.

From Fig. 4a, it was observed that the plume size of hydrogen was comparable to the diameter of the inlet during the initial stages of the leak (10s). Subsequently, at 60s (Fig. 4b), the direction of the leak was downward, while smaller concentrations of hydrogen could be observed towards the top of the box. The downward movement of the gas (and subsequent interaction with the surface) can be attributed to the Coanda effect, and the gas being less dense than air [56]. At 150s (Fig. 4c), it was noted that a small concentration of hydrogen could be measured from the bottom of the box to the top that suggested the presence of hydrogen throughout the whole volume. From Fig. 4e and f, almost no changes are observed in the concentration of hydrogen which was suggestive of the fluid domain being saturated. The lack of venting in the cupboard model limits the diffusion and mixing of gas, resulting in saturation of the fluid domain. It must be noted that in a realistic case a cupboard is likely to have some measure of ventilation, but for the purpose of this study, ventilation has been ignored to allow for observation of gas movement within the cupboard volume.

From Fig. 5a, the key point to note was the spread of the plume towards the edge of the box and trace amounts of methane in the rest of the domain in a very short time frame (10s). Following that, at 60s (Fig. 5b), it was observed that the direction of the leak was downward near the inlet, while the gas could be seen moving upwards. It was also observed that the gas interacted with the lower surface of the box during its movement. At 150s (Fig. 5c), the methane had diffused throughout the

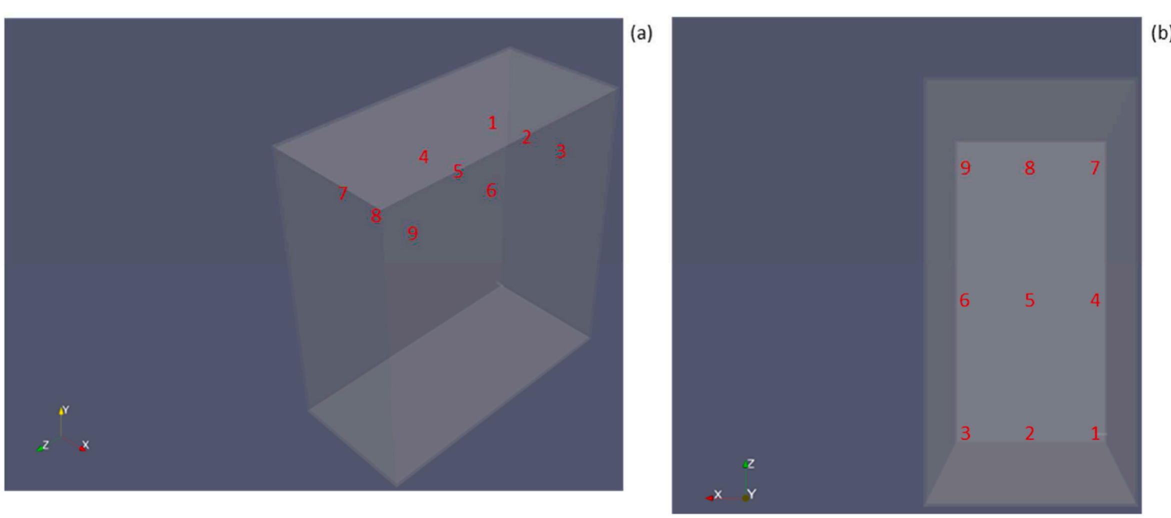

Fig. 3. (a) Isometric view; and (b) Top View of the cupboard geometry to mark the locations of point probes (Labelled 1–9) for gas concentration measurement.

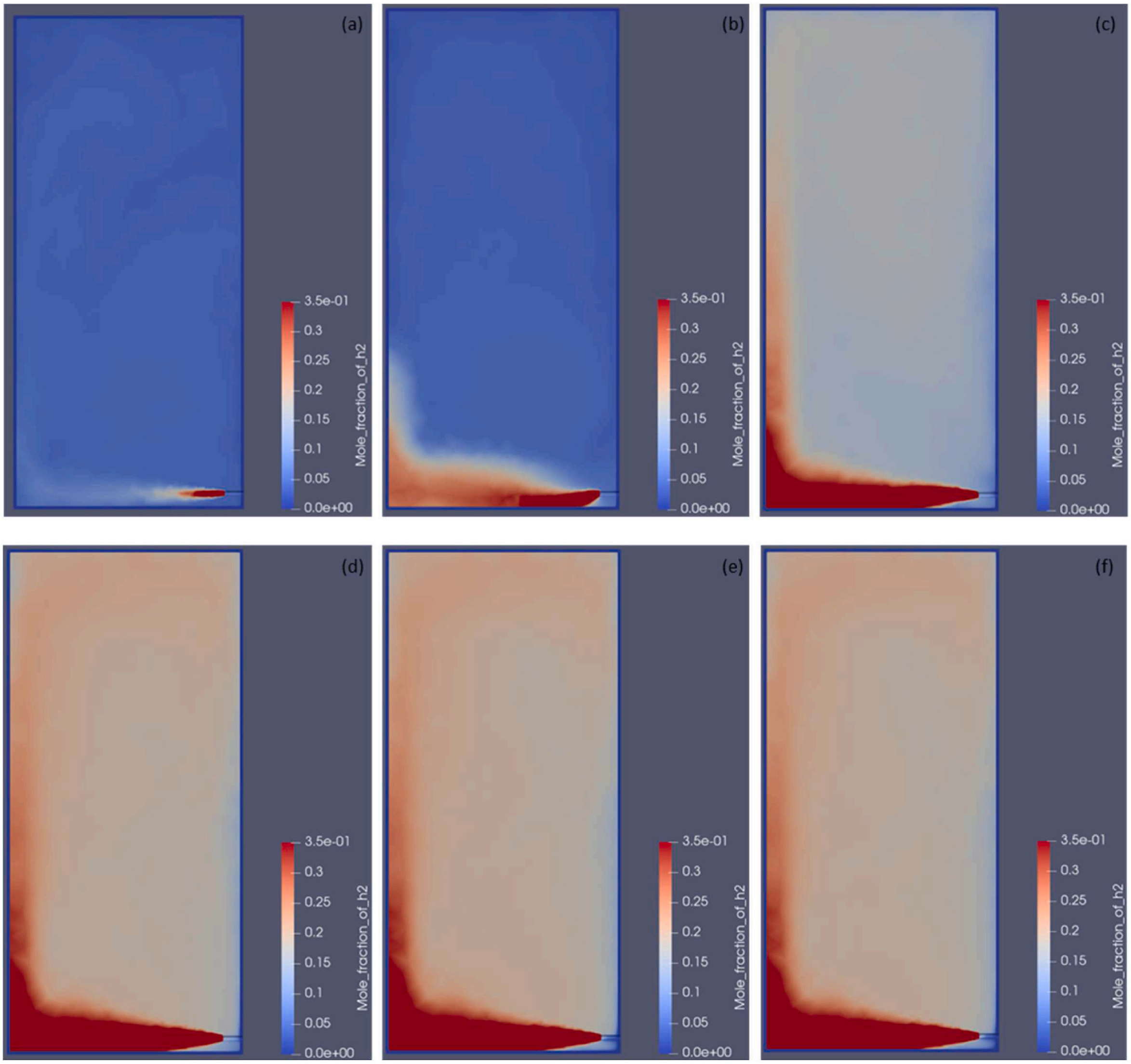

Fig. 4. Leakage of hydrogen gas (gas inlet from the bottom of cupboard at a flowrate of 18.36 m^3/h) based on mole fraction in the fluid domain at (a) 10s; (b) 60s; (c) 150s; (d) 300s; (e) 450s; and (f) 600s. The contour from blue to red shows an increase in mole fraction of the gas from 0 to 0.35 respectively (mole fraction of gas above 0.35 is also represented by red). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

domain with marginally higher concentrations towards the top (ignoring the inlet). At 300s (Fig. 5d) and 450s (Fig. 5e), there was a slight increase in the methane concentration towards the top of the cupboard, suggesting the accumulation of gas in that region. Furthermore, the concentration of methane was largely unchanged at 600s (Fig. 5f), which suggested that the gas had saturated the system.

When observing the leakage of methane and hydrogen into the same domain, their behaviour is qualitatively similar, but there are significant differences quantitatively. While both gases tended to diffuse upwards, hydrogen ends up with a higher concentration in air (approximately 25% in air) at 600s. Methane being the denser, and more viscous gas tended to move downward first, before diffusing towards the top of the cupboard (Fig. 5b, c, and 5d). Based on a visual assessment, methane had more interactions with the surface of the cupboard during the leakage process compared to hydrogen. This resulted in both gases having similar concentrations (8% in air) near the top edges of the domain. At this concentration, both gases are within their flammability limits and there is a risk of accidental initiation, if an ignition source was present. Furthermore, methane had a concentration of about 10% in air, while hydrogen had a concentration of approximately 25% in air when assessing areas away from the boundaries of the domain. These values were also within the flammability range of the two gases, thus highlighting the risk when a gas leak occurs in a small volume.

3.2. Effect of gas inlet and leak diameter

The simulations for leakage of hydrogen and methane were carried out for different leak diameters, and different inlet locations as shown in Fig. 1b. As mentioned earlier, the leak diameters were varied by changing in the hydraulic diameter boundary condition in the simulation setup. This was done to replicate previous experimental work that studied leakage of hydrogen and methane in confined spaces [28]. The location of the gas inlet was considered as a variable to compare both gases because it affects the diffusion of gas within the cupboard volume and influences the interaction of the gas with the solid surfaces of the cupboard. The leak diameter was used to compare the flow of hydrogen and methane into the cupboard fluid domain because changing the diameter affects the volumetric flowrate of the gas. Consequently, this is expected to affect the concentration gradient between the gas inlet and the rest of the fluid domain, thus influencing the diffusion process of the gas within the system. The change in gas concentration of hydrogen and methane with respect to time for different inlet locations and diameters

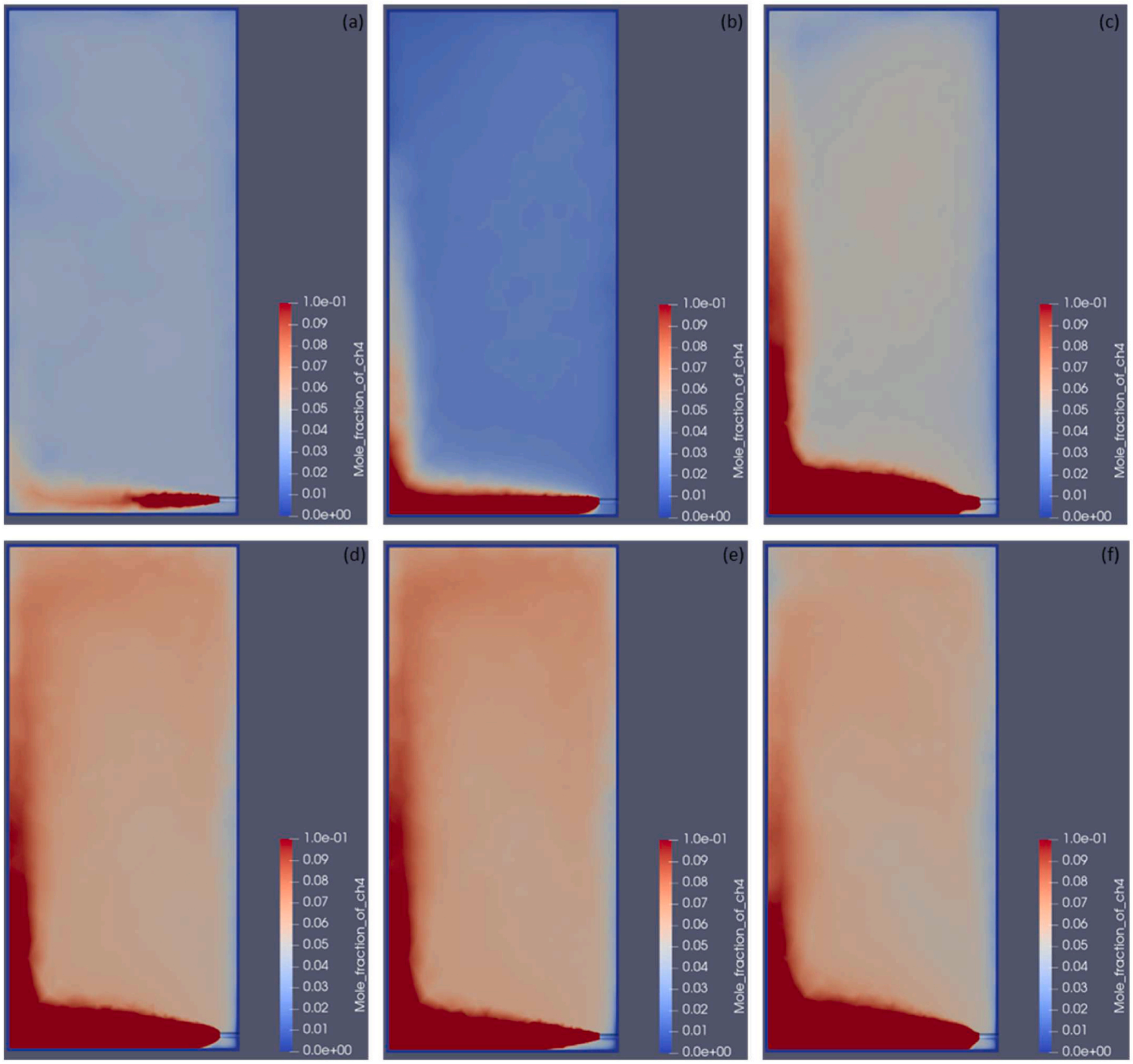

Fig. 5. Leakage of methane gas (gas inlet from the bottom of cupboard at a flowrate of 6.4 m^3/h) based on mole fraction in the fluid domain at (a) 10s; (b) 60s; (c) 150s; (d) 300s; (e) 450s; and (f) 600s. The contour from blue to red shows an increase in mole fraction of the gas from 0 to 0.1 respectively (mole fraction of gas above 0.1 is also represented by red). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

are shown in Figs. 6 and 7, respectively.

From Fig. 6, the key observation was that the inlet diameter directly influenced how the hydrogen leaks into the space and the time it takes for the system to reach equilibrium. Here equilibrium refers to the point in the process where the concentration of gas remains approximately constant (±5% deviation around a fixed value). The concentration of hydrogen at equilibrium was between 20 and 30% in air depending on the inlet location. It was noted that scenarios with leak diameter 7.2 mm reached equilibrium concentration the fastest at around 150s (Fig. 6b, c, 6d, and 6e) and 350s (Fig. 6a and f). This discrepancy could be due to the inlet location relative to the measurement probes, and the effect of turbulent mixing in the system [53]. The same shift in time to reach equilibrium was noted for inlet diameters 5.1 mm and 3.6 mm for Fig. 6a and f. In most cases (except for Fig. 6b), hydrogen does not reach equilibrium concentration for a leak diameter of 1.8 mm because the flow rate is too low. For Fig. 6b, the hydrogen seems to reach equilibrium concentration (25%) due to the inlet location being close to the measurement location and the rapid diffusion upwards. The influence of inlet location on the hydrogen concentration in the box can also be observed in Fig. 6. Cases where hydrogen was entering the box from the middle (Fig. 6b and e) showed a higher equilibrium concentration (25% from Fig. 6b, and 22% from Fig. 6e) as compared to the top or bottom corners of box. A potential reason for this observation is the interaction between the gas and cupboard surfaces during the diffusion process. Cases where the gas had to interact with multiple surfaces during the diffusion process showed a slight delay in time (equilibrium concentration was reached 45s slower in case of a corner inlet as compared to the centre) required to reach equilibrium, and a lower equilibrium concentration (28% lower equilibrium concentration when gas inlet was located near a corner as compared to the centre) at the end of the simulations. It was also noted that the equilibrium concentration was lower for cases where the hydrogen entered the system from the lower end of the box (Fig. 6c and d) as compared to the concentration when the gas entered from higher in the box (Fig. 6a and f). Cases with lower hydrogen entry locations reached an equilibrium concentration of 20% in air compared to high entry locations that reached an equilibrium concentration of 25% in air.

From Fig. 7, it could be seen that the equilibrium concentration for methane in the fluid domain is between 6 and 7.3%, which is much lower than hydrogen. The reason for this is the lower flowrate, and higher mass of methane compared to hydrogen. For all cases in Fig. 7, methane concentration in air reaches equilibrium fastest for cases with

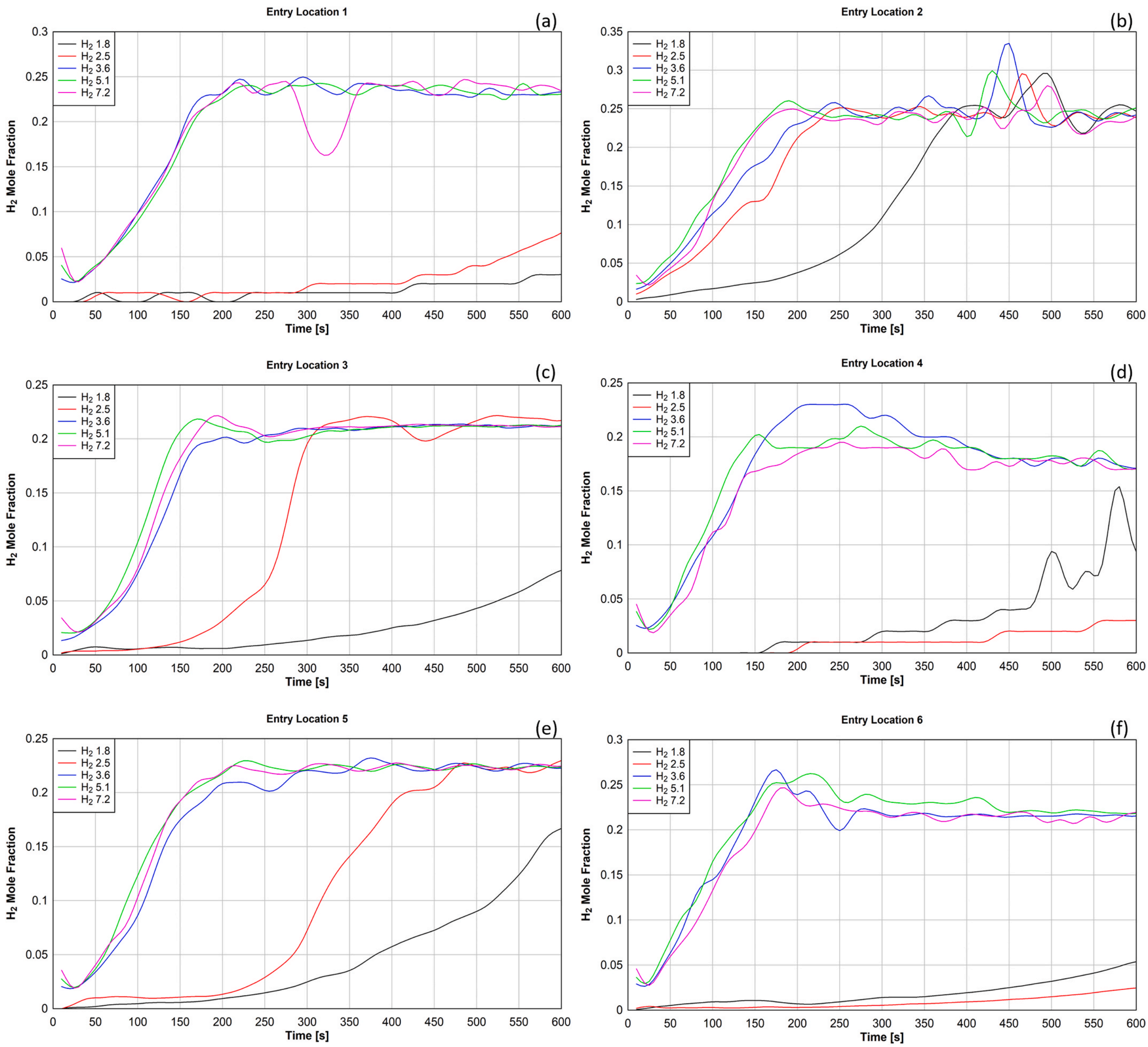

Fig. 6. Change in hydrogen concentration in a cupboard for different leak diameters (1.8 mm; 2.5 mm; 3.6 mm; 5.1 mm and 7.2 mm) at (a) entry location 1; (b) entry location 2; (c) entry location 3; (d) entry location 4; (e) entry location 5; (f) entry location 6 (Entry locations as shown in Fig. 1b).

leak diameter of 7.2 mm. For the 7.2 mm diameter leak case in Fig. 7a, c, 7d, and 7f, the equilibrium concentration is achieved at approximately 235s compared to 150s in Fig. 7b, and 190s in Fig. 7e. The possible reason for this could be the relatively higher viscosity of methane, and the influence of gas-surface interactions on the diffusion process. In most cases (Fig. 7b, d, 7e, and 7f), methane leaking from the 1.8 mm diameter hole does not reach equilibrium concentration due to the low flow rate. Conversely, the methane leaking from the 1.8 mm hole reaches the equilibrium concentration (6.4%–7.3% in air) when the inlet location is at the top or bottom corner (Fig. 7a and c). The potential reason for this could be the increase in turbulent mixing due to the interaction of the gas with two solid surfaces during the leakage process [53,57]. Furthermore, the equilibrium concentration is marginally lower for cases where the methane is entering the fluid domain from lower locations as compared to when it enters from a relatively higher location. The key reason for this is the increased distance between the measurement locations in relation to the inlet locations. The diffusion of gas reduces over higher distances thus resulting in a lower concentration towards the top of the box for the same duration of time.

When comparing the two gases, certain similarities and differences can be observed in their leakage scenarios and the factors influencing the gas transport process. For both cases, the inlet location affected the time taken to reach equilibrium, and the equilibrium concentration at the top of the box. This is because the inlet location defined the number of surfaces that the gas interacted with, which in turn affected its diffusion within the box. Furthermore, the leak diameter influenced the rate at which the equilibrium concentration of gas was reached, and the fluctuations in the measurement of concentration. Larger leak diameters represented cases with higher turbulence in gas flow, resulting in relatively faster diffusion of methane and hydrogen in air. Additionally, it was noted that the higher flowrate of hydrogen compared to methane resulted in the proportionally higher equilibrium concentration in the simulations. For all cases where the leak diameter was 3.6 mm, 5.1 mm, and 7.2 mm, the equilibrium concentration for both hydrogen and

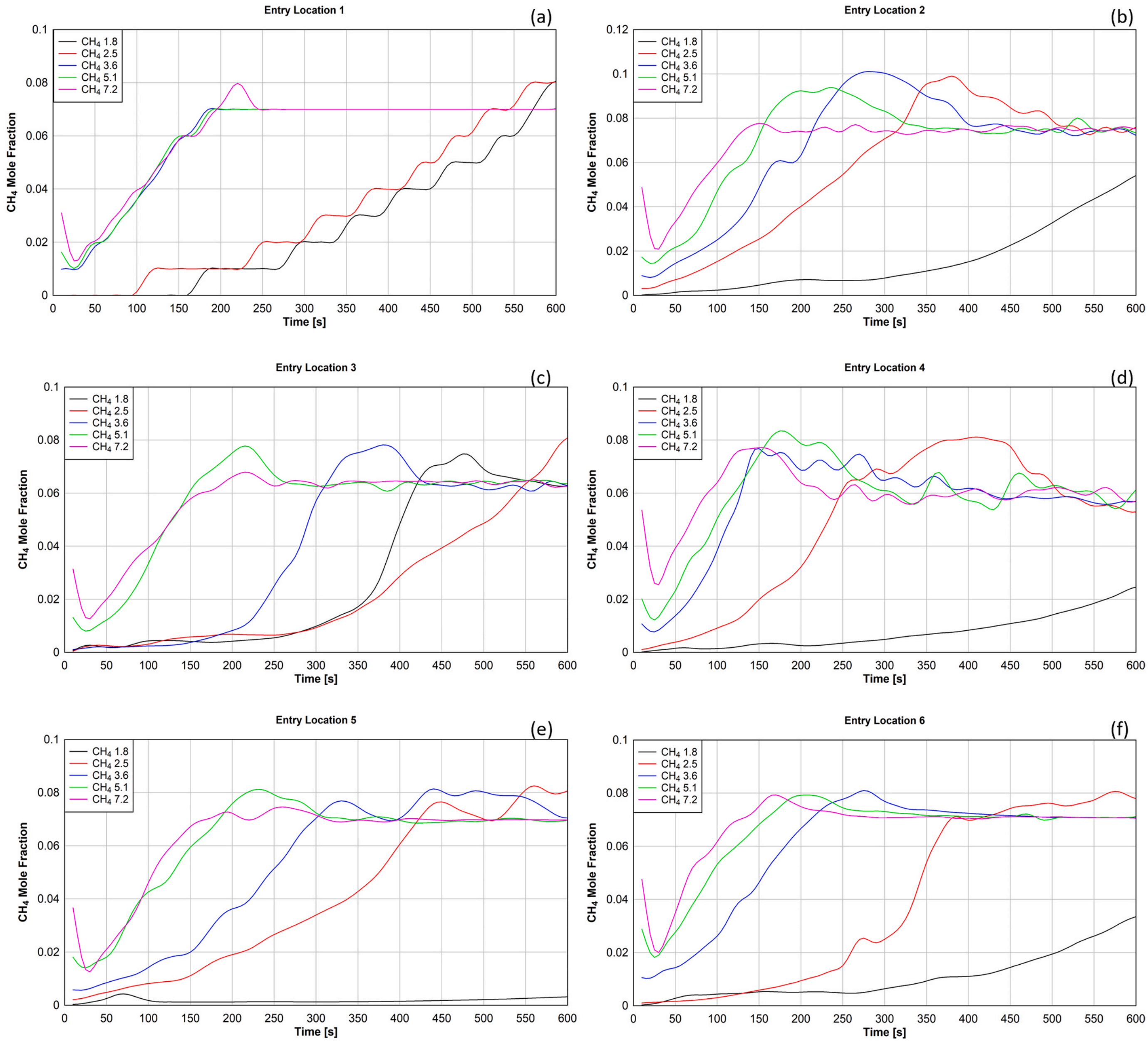

Fig. 7. Change in methane concentration in a cupboard for different leak diameters (1.8 mm; 2.5 mm; 3.6 mm; 5.1 mm and 7.2 mm) at (a) entry location 1; (b) entry location 2; (c) entry location 3; (d) entry location 4; (e) entry location 5; (f) entry location 6 (Entry locations as shown in Fig. 1b).

methane were within their flammability range. For leak diameter 2.5 mm, hydrogen concentration depended largely on the inlet location and surface interactions, and it was not in the flammability range (<4% in air) for entry location 4 and 6 (Fig. 6d and f, respectively). For 2.5 mm leak diameter, methane concentrations were within the flammability ranges for all cases. For 1.8 mm leak diameter, hydrogen concentrations were within the flammability ranges for all entry locations except the top corner (Fig. 6a), even if they did not reach the equilibrium concentration. For the 1.8 mm leak diameter, methane concentrations did not enter the lower flammability limit (5% in air) for cases with 1 boundary surface interacting with the gas (Fig. 7d, e, and 7f). Based on these findings, the risk profiles of hydrogen and methane can be compared for this leakage scenario.

3.3. Comparison to existing work

The modelling study was designed in accordance with previous experimental work carried out during the Hy4Heat projects [28]. However, certain changes were made in the simulation methodology due to differences in the experimental setup and the model design. The experimental work was carried out for measuring the leakage for a whole house, while the modelling was done for a gas leak in a wall cupboard without venting. Consequently, the timescale for the models was also reduced to 10 min (600s) instead of 250 min (15000s).

Considering these differences in the methodology, the findings from the modelling study broadly align with the results of experimental work. The key observation to support this claim is the change in gas concentration. In the experimental study, and the simulations, the common trend was a sudden rise in gas concentration over a short period of time before it reached an equilibrium value. A similar trend is noted in the simulation results as observed in Figs. 6 and 7. In addition to this, the experimental study proved that both methane and hydrogen tend to accumulate and stratify towards the top of confined spaces as they leak and diffuse from a single point of entry. Based on Figs. 4 and 5, it can be confirmed that the same observations were made from the modelling study as well.

3.4. Qualitative assessment on the risk profile of hydrogen

Based on this study, certain qualitative assessments can be made regarding the risk of using hydrogen for domestic applications. Given the trends in hydrogen leakage in confined spaces, the key sources of risk are its low ignition energy, and wide flammability range [58]. Consequently, in the case of an ignition event, it is known that hydrogen has a high burning velocity, high temperature, and poses a detonation risk under specific conditions [59,60]. Based on how hydrogen diffuses in a closed volume, it is relatively easy to predict trends in gas concentration, thus creating the opportunity to put in place viable systems for leak detection and accident prevention. In case of a leak, it is known that hydrogen tends to stratify, resulting in the formation of high-level flammable vapour clouds. While this might be considered a high-risk situation, it can easily be prevented with the use of gas venting systems. When compared to methane, the use of hydrogen poses similar risks, but requires more control measures due to its increased sensitivity. However, the development of early detection methods can allow for mitigating the risk posed by hydrogen. The use of visual sensors, and odorants can enable early detection of hydrogen, thus reducing its risk to current safety standards [61–63].

4. Conclusion

Numerical modelling was done to assess the leakage of hydrogen and methane in confined spaces. The control volume selected was used to represent a kitchen cupboard along with 6 different leak locations and a range of leak diameters (1.8 mm–7.2 mm). The leak diameters were selected to represent different scenarios based on increasing severity of consequence in a leakage scenario. The leakage of hydrogen and methane into the confined space was compared based on the leak diameter and the leak location. The key findings of this study were:

- Hydrogen and methane both tend to move upwards during the diffusion process and tend to stratify towards the top of a given space. The diffusion of the gas in the fluid domain is affected by its interaction with the surfaces of the cupboard.
- It was found that the leak diameter is inversely correlated with the time taken for the gas to reach equilibrium concentration within the control volume.
- In the case of hydrogen leakages, the leak diameter influences the flowrate of gas coming into the cupboard, and thus the time taken for the gas concentration to reach equilibrium. It was observed that gas leaking from a 7.2 mm diameter hole reached maximum gas concentration 25s–300s faster than leakages from 2.5 mm holes.
- Like hydrogen, the leak diameter influences the time taken for the methane to reach equilibrium gas concentration in a closed space. It was observed that gas leaks from a 7.2 mm diameter hole reached maximum gas concentration up to 310s faster than leakages from 2.5 mm holes.
- Under severe conditions (gas leakage from 7.2 mm holes), it was observed that hydrogen reached the equilibrium concentration up to 45s faster than methane.
- It was noted that the inlet location of the gas influenced the equilibrium concentration for the system. In the case of hydrogen, simulations with inlet locations near the corners had up to 28% lower equilibrium concentrations than locations near the centre of the cupboard.
- In the case of methane, simulations with inlet locations near the corners had up to 25% lower equilibrium concentrations than locations near the centre of the cupboard.

Future work based on the findings of this study will look to model the leakage of gas in more complex geometries to represent a more realistic scenario. Follow on work will also aim to model the combustion of hydrogen in a confined space to understand the effect of confinement on hydrogen deflagration and the subsequent risk it poses. Lastly, parametric studies following the current work will look at the influence of temperature, moisture, and obstacles on the leakage of gas within a small, confined space.

In conclusion, it must be noted that hydrogen has the potential to be used in a domestic setup. The potential of its use must be caveated using systems to adequately detect and mitigate hydrogen leakages before it enters its flammability range. Lastly, measures must be put in place to minimize the risk of any stimuli interacting with hydrogen during a leak to ensure no accidental initiation occurs.

Funding

The work was supported by Cranfield University and DNV Energy Systems, UK.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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