A MULTI-ZONE MODEL FOR HYDROGEN ACCUMULATION AND VENTILATION IN ENCLOSURES

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ABSTRACT

Due to the small characteristic molecular size of hydrogen, small leaks are more common in hydrogen systems compared to similar systems with hydrocarbons. This, together with the high reactivity, makes an efficient ventilation system very important in hydrogen applications. There are several models available for ventilation sizing that are based on either a well-mixed assumption or a fully stratified situation. However, experiments show that many realistic releases will be neither, and therefore additional models are needed. One possibility is to use CFD-models, but the small release sizes for pinhole releases (<<1 mm) make it difficult to find an appropriate mesh without excessive computational time (especially since the simulations need to be iterated to find the optimum ventilation size). An alternative approach, which is described and benchmarked in the current paper, is to use a multi-zone model where the domain is divided into several large cells where the mass exchange is simplified compared to CFD, and thus simulation time is reduced. The flow in the model is governed by mass conservation and density differences, due to concentration gradients, using the Bernoulli equation. The release of gas generates a plume which is modelled based on an empirical plume model which gives the entrainment and hydrogen source term for each cell. The model has a short run time and will therefore allow optimization in a short time frame. The model is benchmarked against five experiments with helium at the Canadian Nuclear Laboratories (CNL) in Canada and one hydrogen experiment performed at Lodz University of Technology in Poland. The result shows that the model can reasonably well reproduce accumulation in the experiments with small release without ventilation, but appears to slightly underestimate the level of stratification and the interface height for ventilated cases where the source is elevated from the floor level.

The software presented in this paper is freely available at: https://doi.org/10.5281/zenodo.8037661

1.0 INTRODUCTION

When hydrogen is released in an enclosure, various levels of stratification can be obtained as illustrated in figure 1. For low-velocity releases in unventilated enclosures, a relatively distinct layer can be expected [1], while higher plume velocities promote mixing, leading to a well-mixed or gradient situation [1, 2]. The presence of ventilation generally promotes an increased difference in concentration between bottom and top part of enclosure.

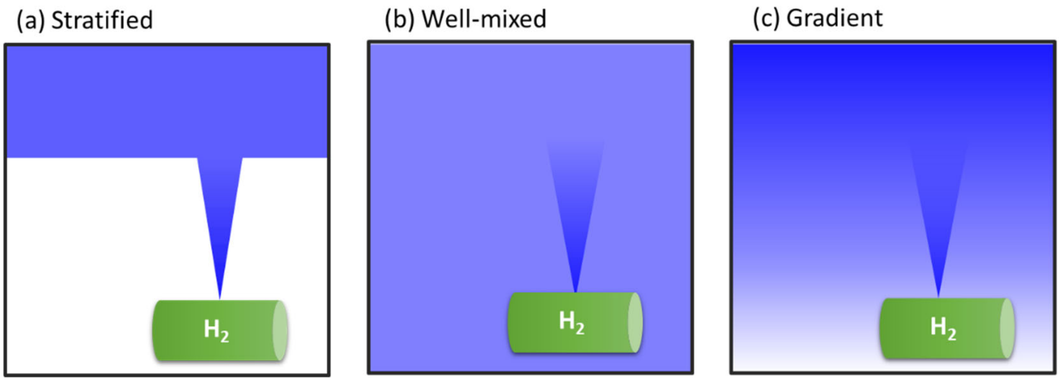

Figure 1. Modes of hydrogen accumulation in enclosures

Since predicting hydrogen accumulation and convection is important for vent sizing, several models have been proposed. The most validated model is the model by Linden [3], which is based on stratified conditions and was later extended to include wind effects by Lowesmith et al. [4].

A model based on the well-mixed distribution was developed by Prasad [2], accounting for multiple vents and both natural and forced ventilation, and well-mixed model is also the basis for the background concentration for ATEX-applications [5].

For the gradient situation, Barley et al. [6] developed an analytical expression for the steady-state distribution based on experimentally determined parameters that were later further validated in Barley et al. [7]. There is also a three-zon-model developed by Cleaver et al. [8], where the height is divided into an upper uniform layer, a middle layer with a constant gradient, and a lower with ambient concentrations. Apart from these models, CFD-models are often needed to predict the actual distribution, and this can sometimes be challenging since the leak sizes considered for ventilation sizing is typically very small (e.g. often 0.1 mm^2 according to EN 60079-10-1:2015 [5]), putting high requirement on the mesh resolution in the release.

For unventilated enclosures, the mode of distribution can be estimated using the modified Richardson number described in equation (1), where the stratified case is characterized by Ri>3 the well-mixed by $Ri<2.5\cdot10^{-3,}$ and the gradient case in between [9].

$$Ri = \frac{V^{1/3}g}{U^2} \tag{1}$$

In the equation, V is the enclosure volume, g is the gravimetric constant and U is the characteristic velocity of the leaking gas. Further, stable stratification can be expected when the condition below holds, according to Peterson [10].

$$\frac{H_{sf}}{d_{bjo}} Ri_{bjo}^{1/3}\left(1+\frac{d_{bjo}}{4\sqrt{2}\alpha_T H_{sf}}\right) > 1 \tag{2}$$

In the equation, H_{sf} is the height of the enclosure, d_{bjo} is the orifice diameter, $\alpha_T=0.05$, and Ri_{bjo} is the jet Richardson number according to below.

$$Ri_{bjo} = \frac{(\rho_a-\rho_0)g d_{bjo}}{\rho_a U_0^2} \tag{3}$$

In the equation, ρ_a is the ambient density, ρ_0 is the density of the leaked gas, and U_0 is the characteristic velocity of the release.

According to Kotchourko et al. [11], the gradient case is not yet fully understood, which may lead to the risks of such systems being underestimated. This is due to the fact that concentration gradients generally increase the probability of the flame reaching areas associated with higher (laminar) burning velocities. Also, the gradients in themselves promote strong flame acceleration through density differences, potentially leading to (quasi-) detonation.

In this paper, a new model for hydrogen accumulation and ventilation sizing is developed and benchmarked. The model is based on the multi-zone concept, which has previously been applied to study the spread of combustion products from fires in enclosure fires with good results [12].

2.0 THE MULTI-ZONE MODEL

The fundamental principle of the multi-zone model is that the enclosure is divided into several regions (horizontal) and layers (vertical) representing multiple computational zones. A schematic representation is shown in Figure 2.

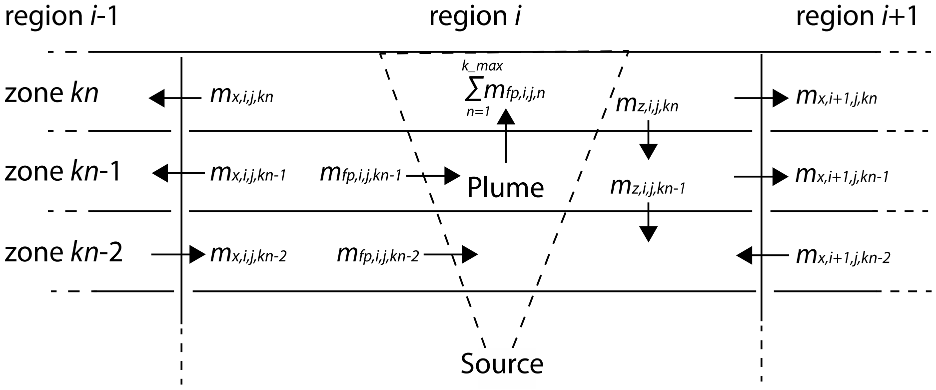

Figure 2. Principles of the multi-zone concept redrawn from Suzuki et al. [13]

Each computational zone has uniform species concentration and operates with conservation of mass. The difference in concentration generates density differences between zones which result in pressure differences that drive the flow between the cells according to the principles of the Bernoulli equation. Diffusion of the studied gas is modelled in accordance with Fick's law.

The release of gas generates a vertical plume, and, as the plume passes through the different zones, air from that layer is entrained. Turbulence in the zones is neglected, but the turbulence in the plume is included through the empirical plume model.

The conservation equation for mass in a zone is as follows:

$$\frac{d}{dt}\left(\rho_{i,j,k}V_{i,j,k}\right)=-\dot{m}_{fp,i,j,k}+\dot{m}_{x,i-1,j,k}-\dot{m}_{x,i,j,k}+\dot{m}_{y,i,j-1,k}-\dot{m}_{y,i,j,k}+\dot{m}_{z,i,j,k+1}-\dot{m}_{z,i,j,k} \tag{4}$$

where $\rho_{i,j,k}$, [kg/m^3] and $V_{i,j,k}$, [m^3] are the density and the volume of the *k*-th layer in the region with x-coordinate *i* and y-coordinate *j*, and $\dot{m}_{fp,i,j,k}$ [kg/s] is the mass flow rate entrained into the plume in that zone. The horizontal mass flow rate from the (i-1)-th and (j-1)-th region to the i-th and j-th region is represented by $\dot{m}_{x,i-1,j,k}$ and $\dot{m}_{y,i,j-1,k}$ respectively. The horizontal mass flow rate from the k-th down to the (k-1)-th is $\dot{m}_{z,i,j,k}$. The total plume mass flow enters the top layer in each region; furthermore, there is no layer above the top layer, this means that the conservation of mass for the top layer becomes as follows:

$$\frac{d}{dt}\left(\rho_{i,j,k\_max}V_{i,j,k\_max}\right)=$$

$$\sum_{n=1}^{k\_max-1}\dot{m}_{fp,i,j,n}-\dot{m}_{z,i,j,k\_max}+\dot{m}_{x,i-1,j,k\_max}-\dot{m}_{x,i,j,k\_max}+\dot{m}_{y,i,j-1,k\_max}-\dot{m}_{y,i,j,k\_max} \tag{5}$$

If there is no gas release in the region, the plume entrainment, $\dot{m}_{fp,i,j,k}$, will be zero.

The equation to calculate the plume entrainment used in the model has previously been applied by Prasad and Yang [14]. The equation predicts that the volumetric flow rate $\dot{Q}$ in the plume in an un-stratified environment varies as a function of height *z* measured above the release point as,

$$\dot{Q}(z) = \frac{6\varepsilon}{5}\left(\frac{9\pi^2\varepsilon}{10}\right)^{1/3} B_0^{1/3}(z + z_0)^{5/3} \tag{6}$$

Where the entrainment constant, ε, is set to 0.102. The flow rate of buoyancy, B_o, is related to the volumetric flow rate of hydrogen, and z_o, represents a virtual origin of the source. Equation 6 describes a bouancy driven plume which will have different behaviour compared to a momentum driven jet. There are methodologies based on the Froude number at the source that can be used to quantify at what distance a momentum-dominated jet is transferred into a bouancy-dominated plume [15]. Such a methodology is applied to controlled that Equation 6 is applicable. It was demed sutiable to use this kind plume model due to the relatively small releases studied. Indeed, a 0.1 mm^2 leak, which is common in ATEX-applications and also relevant for ventilation sizing, will be fully buoyancy dominated, according to this criterion, already after 0.09 m even at 500 bar. This implies that entrainment the buoyancy dominated region is important in actual applications, but this should be put under scrutiny in future developments and validations.

Ventilation openings of different size and positions can be added in the model. Only one opening can be added to each vertical face of zones that are in contact with the exterior boundary of the domain. A discharge coefficient of 0.8 is applied.

The multi-zone model developed for this work is based on a model that was developed for smoke filling and temperature calculations of large volumes [12]. The model has no graphical user interface and runs from an executable file that reads a text input file.

3.0 EXPERIMENTS

The model is benchmarked against two sets of experimental data in the published literature covering, in total, six cases. Among the six cases, helium was used as a surrogate gas in five.

3.1 Experimental data sets

The first dataset is based on data from a series of helium dispersion tests in an empty semi-confined enclosure and has been performed by Liang et al. [16] and Liang et al. [17]. The tests were conducted in an enclosure with a total volume of approximately 16.6 m^3 (2.6 m (l) × 2.6 m (w) × 2.45 m (h)). The enclosure was constructed from aluminum beams and polycarbonate sheets. The connections between walls, floor and walls and ceiling and wall were sealed to minimize leakage.

In both test series, helium was released from the center of the enclosure with a nozzle (Ø = 2.5 cm) pointing upward and located 10 cm above the floor. In the first series [4], there was one circular vent (Ø = 5 cm) open in the floor about 20 cm from the center of one of the side walls. In the second series [5] there were three openings on the side walls, one upper vent (V_2) placed 20 cm below the ceiling and two lower vents (V_1 and V_3) placed 10 cm above the floor. Each vent had a diameter of 11.4 cm. In the first test series, six tests were performed where the injection flow rate was varied between the tests. In the second test series, the injection rate, the elevation of the injection, wind effect on vents and size of vents were varied. The cases with wind were not included in the benchmark since the model currently does not include capabilities to account for wind.

The second data set was published by Brzezińska [18], who performed two experimental tests with hydrogen release in a confined 60m^3 (approximately 5 m (l) × 4 m (w) × 3 m (h)) large room. The hydrogen release was 1.63×10^{-3} m^3/s in both tests, but the type of release source varied (single nozzle with Ø = 0.4 cm and multi-point release). Only data from the single nozzle test is used in this paper. Hydrogen concentrations over time at three elevations (0.4, 1.4 and 2.9 m) are given in the paper.

Information about the tests used for benchmarking of the MZ model is presented in table 1.

Table 1. Description of the tests used in this study to benchmark the MZ model.

Test	Gas	Room volume *[m^3]*	Nozzle diameter *[mm]*	Mass flow *[g/s]*	Floor vent diam. *[cm]*	Top vent diam. *[cm]*	Source height above floor [m]	Reynolds number [-]	Richardson number [-]	Ref
1	He	16.6	25	0.0028	5	- *	0	15	5427	[16]
2	He	16.6	25	0.0698	5	- *	0	363	9	[16]
3	He	16.6	25	0.0140	11.4	11.4	0.1	73	217	[17]
4	He	16.6	25	0.0140	11.4	11.4	1	73	217	[17]
5	He	16.6	25	0.0140	11.4	11.4	1.7	73	217	[17]
6	H_2	60	4	0.137	- **	- **	0	27740	0.0015	[18]

* Liang et al. [16] acknowledges that there were distributed leaks in the enclosure used in the experimental tests. This is accounted for in the setup of the numerical model the same way as in the original publication.

** Brzezińska [18] acknowledges that there were leaks in the enclosure used in the experimental tests. This is accounted for in the setup of the numerical model the same way as in the original publication.

As can be seen in table 1, test 1-5 is buoyancy dominated, and Richardson number predicts stratified conditions while test 6 is momentum dominated and with a Richardson number predicting well-mixed conditions. However, according to the methodology refered to by the HSE [15] the flow in test 6 will be in an intermediate state between jet and plume at 0.2 m and fully buoyancy-dominated at 1.8 m above the source. Equation (2) from Peterson [10] predicts stable stratification for all cases since the minimum value is 9.8 (for test 6) and minimum 42.3 (for test 1-5).

3.2 Setup in the numerical model

The first experiments by Liang et al. [16] were modelled with a total of 90 (3 × 3 × 10) zones in a domain that was 2.6 m × 2.6 m × 2.45 m. The release was placed on the floor and modelled with a nozzle and mass flow according to the data in Table 1. Liang et al. [16] recognizes that the enclosure is not leak-tight, and in the modelling done in the paper, Liang et al. assumes the bottom vent to have an effective diameter of 5.7 cm and the flow through distributed leaks in the upper part of the enclosure were assumed to correspond to an upper vent with the same effective diameter as the bottom vent. The same treatment of the leaks was applied in the setup of the MZ model used in this paper.

The second experimental series [17] was performed in the same enclosure as the first; thus, the domain was modelled in the same way for Test 3-5 as in Test 1-2. The release was placed and modelled according to the data in Table 1. The discharge coefficient was set to 0.61, which also was used by Liang et al. [17]. The ambient temperature in Test 1-5 was set to 21°C, and the diffusion coefficient of helium was set to 0.0000697 m^2/s.

The third experimental series [18] was modelled as an enclosure with the dimensions 4.9 m (l) × 3.9 m (w) × 3 m (h). A total of 90 (3 × 3 × 10) zones were used in the domain. The release was placed on the floor in the centre of the enclosure and modelled according to the data in Table 1. In the modelling done by Brzezińska [18], leaks in the enclosure are accounted for by introducing a 0.0025 m^2 vent on the floor, a similar vent is added in the MZ model. The ambient temperature was 10°C, and the diffusion coefficient of hydrogen was set to 0.0000756 m^2/s.

The choice of the number of control volumes was based on previous experience from using the approach for fire modeling. No systematic sensitivity analysis on this parameter was performed, but should be examined in future publications.

4.0 RESULTS

Results from modeling are presented together with data from the different experimental tests in the following sections.

4.1 Helium dispersion tests (Test 1-5)

Results from the modeling of the helium dispersion tests performed by Liang et al. [16] (Test 1-2) and Liang et al. [17] (Test 3-5) are presented in this section.

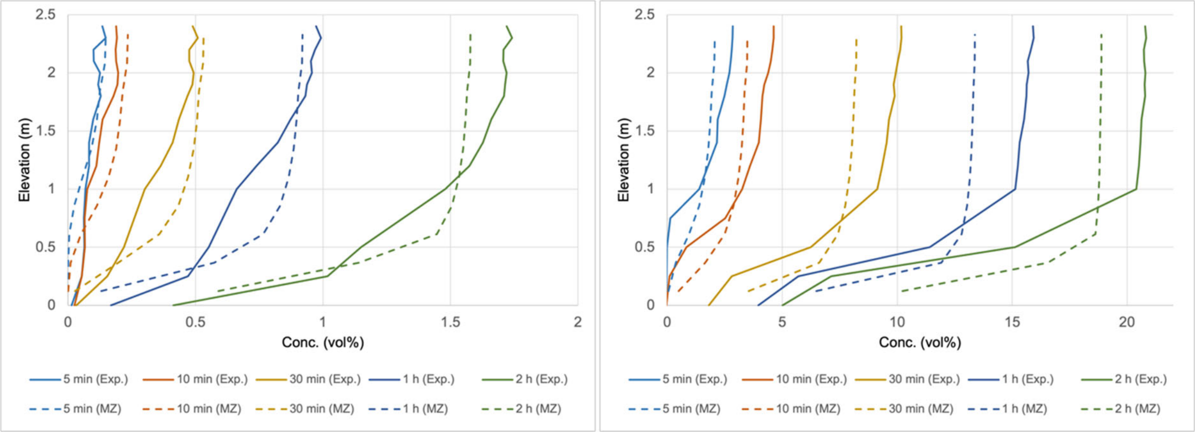

Figure 3. Vertical gas concentration in Test 1 (left) and Test 2 (right).

Reasonable fit to the experimental data; however, concentration underpredicted for the larger release (Test 2).

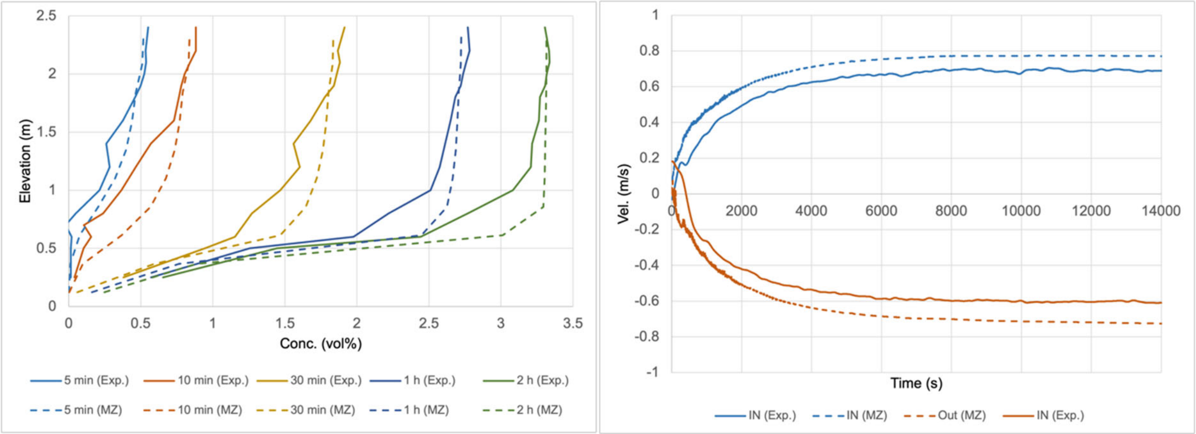

Figure 4. Modeling results from Test 3. Vertical gas concentrations (left) and vent velocities (right).

Reasonable fit to the experimental data both in terms of gas concentrations and gas velocities in the two vents.

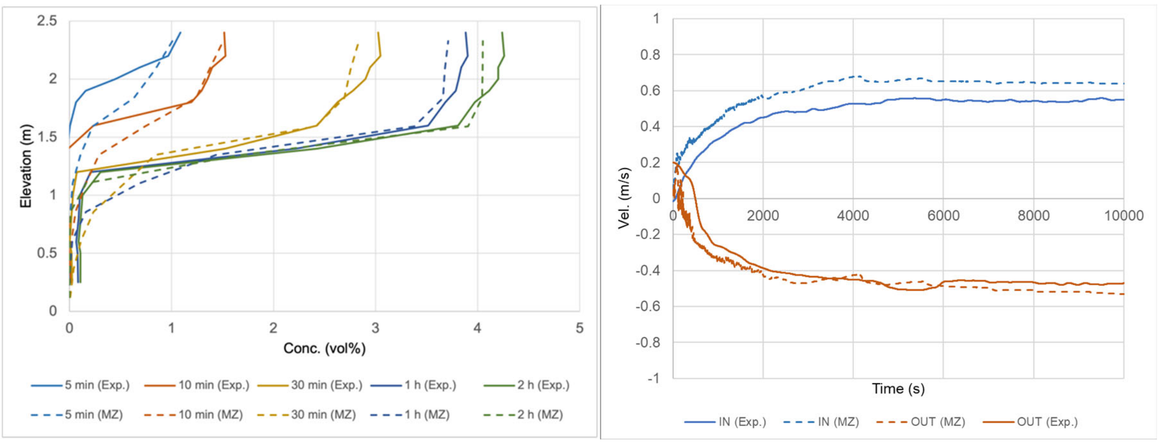

Figure 5. Modeling results from Test 4. Vertical gas concentrations (left) and vent velocities (right).

Reasonable fit to the experimental data both in terms of gas concentrations and gas velocities in the two vents.

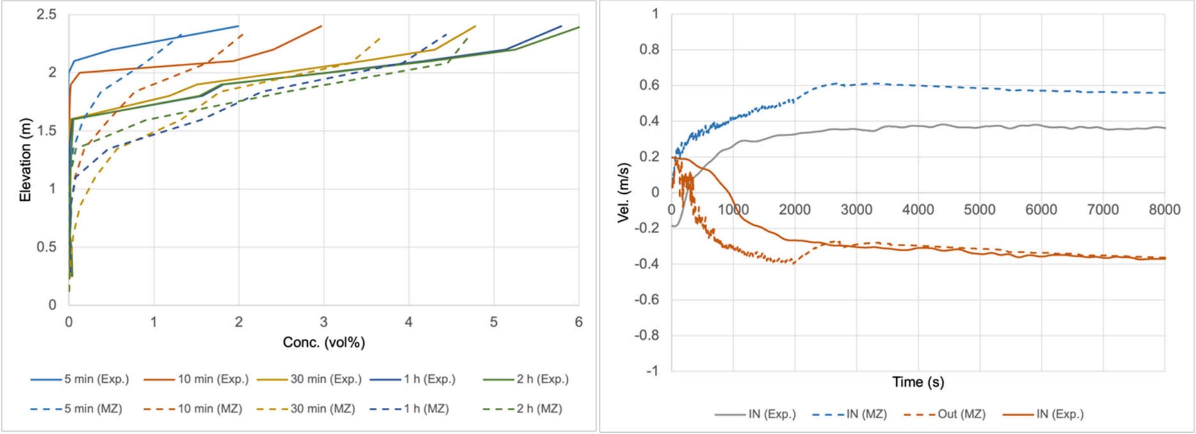

Figure 6. Modeling results from Test 5. Vertical gas concentrations (left) and vent velocities (right).

The right figure in Figure 6 indicates that there are some numerical instabilities in the solution. This is possibly due to the few zones that the plume travels through from the release at 1.7 m to the ceiling. Therefore, the height of the zones used in the MZ model has been reduced to investigate its effect on the results of Test 5, and the results of a simulation with 180 (3 × 3 × 20) zones in MZ are presented in Figure 8.

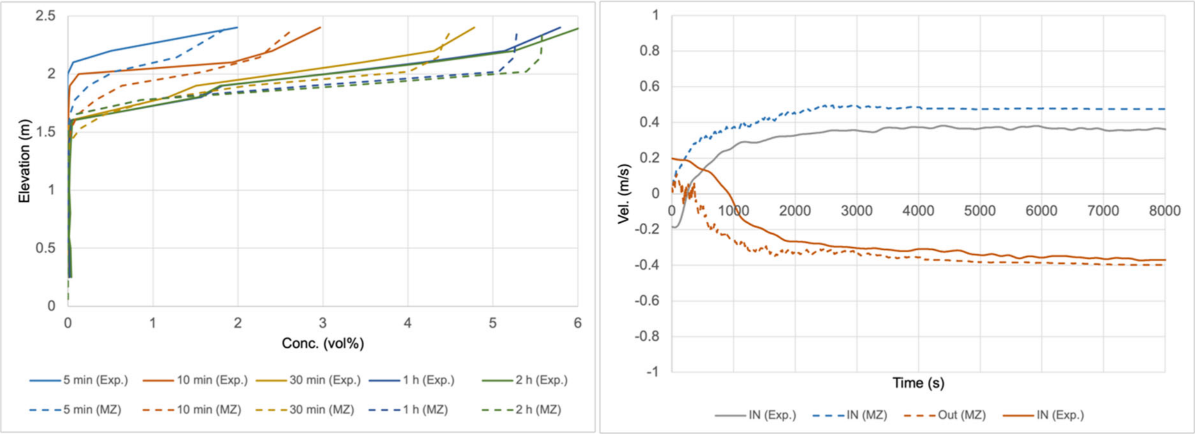

Figure 7. Modeling results from Test 5 with 20 zones in z-direction. Vertical gas concentrations (left) and vent velocities (right).

As can be seen in Figure 7, the increase in vertical resolution shows improved results compared to the cruder resolution presented in Figure 6.

4.2 Hydrogen dispersion tests (Test 6)

Results from the modeling of the hydrogen dispersion test performed by Brzezińska [18] (Test 6) is presented in this section.

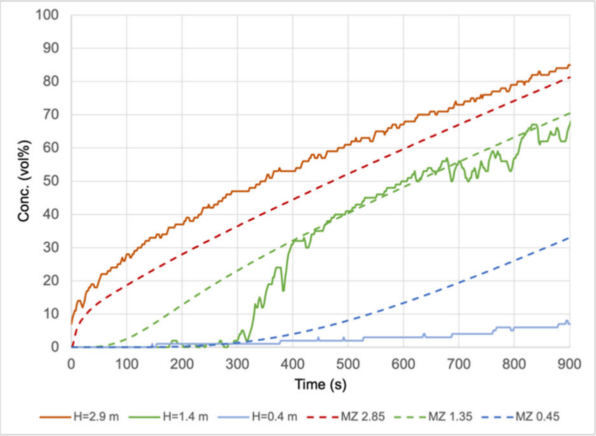

Figure 8. Vertical gas concentrations from Test 7. Dashed lines are from simulation and continuous lines from experiments.

The model underpredicts the concentration close to the ceiling, but captures the general trend. The time to reach down to 1.4 m above floor level was underpredicted. Significant hydrogen concentration was also, in contrast to experiments, found near the floor level.

5.0 DISCUSSION

5.1 Assessment of the accuracy of the model

For the unventilated cases (Test 1-2 – Fig 3), the model appears to give reasonable results for the smaller release while it underpredicts the maximum concentration for the larger release. One reason could be the uncertainties associated with the leaks in the enclosure, which were estimated to be 5 cm in diameter in the paper, based on some modelling work. Since the calculation in the paper was based on a uniform layer, the calculation method was appropriate for the type of model applied, while it might not be appropriate for the current paper. As a sensitivity study, a simulation with a 50 % reduction in the leak area was performed, but the results were inconclusive, with some data points improving and some deviating more from the experimental results. Also, the distribution of leaks over height can be one source of uncertainty.

MZ seems to model the first ventilated case, with release near the floor, well (Test 3 – Fig. 4). Also, the fact that the velocities through the vents are predicted well gives credibility to the results.

The slightly elevated case (Test 4 – Fig. 5) is also modelled well, although the experimental data shows a clearer stratification. These trends are becoming more evident as the source is elevated even higher up (Test 5 – Fig. 6). However, an increase in vertical resolution significantly enhances the predictive capabilities of the model (Fig. 7).

The modelling of actual hydrogen dispersion was limited to only one test (Test 6 – Fig. 8). The gas concentrations at high elevations are under-predicted by MZ, but the concentration development over time is corresponding rather well with the experimental data. The concentration closest to the ground is overpredicted, while the mid-height values are well captured after 400 seconds. One reason for the differences may be that the flow closest to the source is momentum driven, which the implemented dispersion model (Equation 6) does not take into account.

A lack of information about the experiment might have contributed to inaccuracies in the actual setup of the scenario in the MZ model. The description of the experimental setup is crucial to perform a fair benchmarking. The experiments by Liang et al. [16] [17] (Test 1-5) are well described even though there are uncertainties in the amount of leaks in the used enclosure. The setup in the hydrogen dispersion test [18] (Test 6) was not as well described, and the enclosure leaks were modelled as a vent in the bottom of the enclosure since no other data on leaks was available.

5.2 Potential uses of the model

Although the model has not yet been fully validated, it is relevant to consider potential uses of the model. The most obvious is probably vent sizing studies, where many simulations with variations in ventilation (natural or forced) can be applied, and the concentration distribution can be compared against a suitable criterion. The current model is only capable of optimizing for a threshold in maximum hydrogen concentration (e.g. LFL 4% or LHL 8%), but an interesting development would be to combine it with the work on inhomogeneous deflagrations by Makarov et al. [19], where criteria for overpressure in case of igntion could be set.

Further use could be to perform multiple simulations with a fixed ventilation rate, but variation in leak size, location and direction. This could be used in a QRA framework to investigate the probability that a flammable could, large enough to damage the structure, would arise from various small releases. It should however be noted that the model currently only is able to model vertical releases so this requires extension of the dispersion model used.

Finally, the use of the model for optimization of detector placement could be considered. If the enclosure is divided into a higher number of regions (i.e. divisions in the horizontal plane), the distribution of hydrogen in the horizontal plane should in principle be possible to model since this has been achieved for fires [12]. Combined with information about the distribution of components in the enclosure, a similar approach as described in the previous paragraph could be tested to derive a probability distribution of detection times and optimize this on some criteria (e.g. average detection time or 95%-percentile detection time).

6.0 CONCLUSION AND FUTURE WORK

Although some discrepancies between the six experiments and the results from the MZ-model could be found, the overall approach appears fruitful and able to fill a gap between simple algebraic models and full CFD. The short runtime permits both optimization of vent sizes and the possibility of applying the model in a Monte-Carlo based framework for use in QRA or detector placement studies.

However, significant work remains until full confidence can be given to the model. The model should be applied to more well-controlled experiments in the literature, and thorough grid independence studies should be conducted. The model should also be further developed to include models for non-vertical release and wind-effects. It can also be investigated how other types of dispersion models can be implemented and used based on if the release is dominated by buoyancy or momentum. Also, an option of using a more elaborate criterion for minimum ventilation based on explosion overpressures should be included.

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