



Numerical modelling of LH₂ leaks within tank/transfer connection spaces

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Partners



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Contents

This presentation will cover:

- Problem description
- Geometry and meshing
- Physics setup
- Results
- Further work

Modelling problem description

Aim:

- Develop a numerical model capable of capturing dispersion of small releases of liquid hydrogen into an enclosure

Objectives:

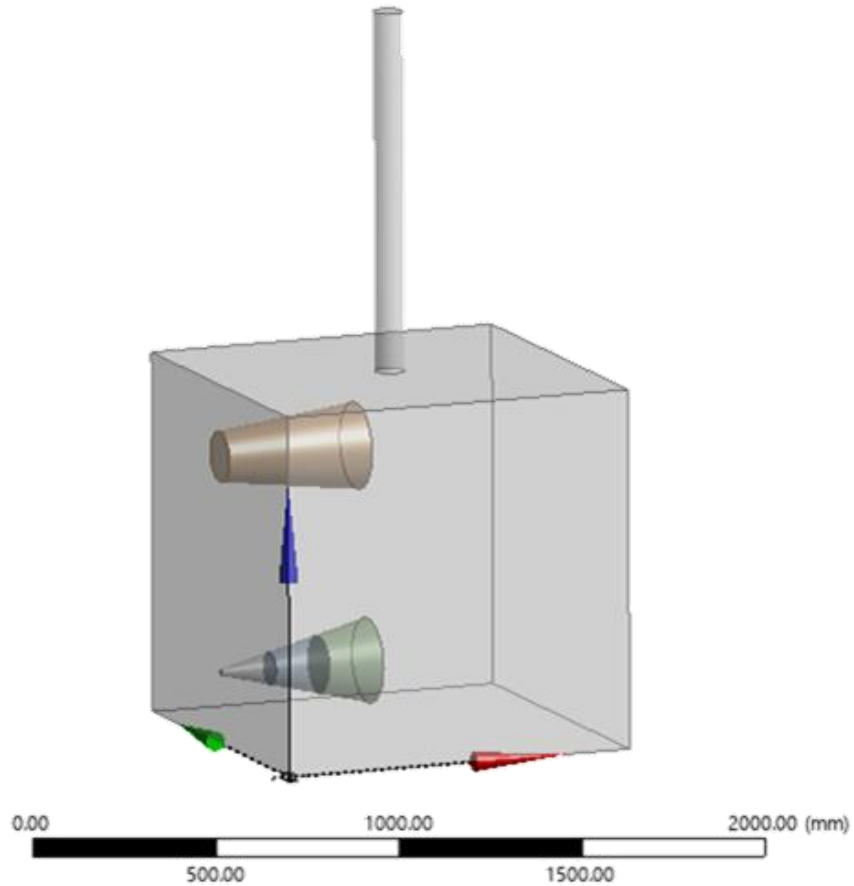
- Review modelling approaches and potential experimental datasets
- Construct model to compare to ELVHYS Task 4.2 experiments
- Investigate model sensitivity to model parameters



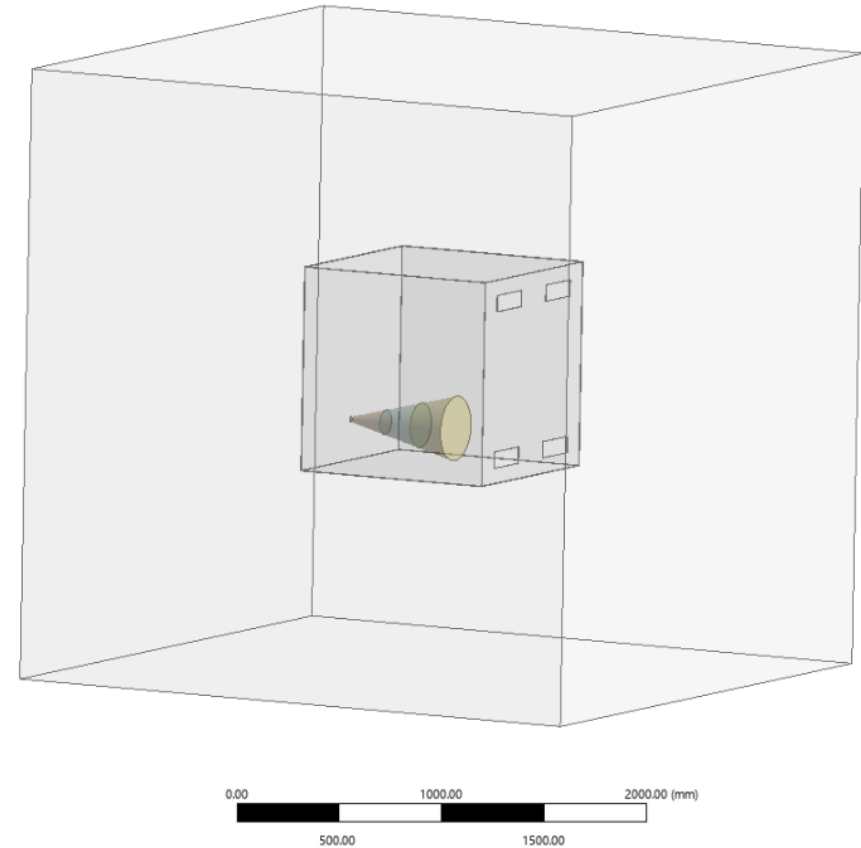
Image taken from an experimental passive ventilation test video

Geometries

- Separate geometries for active ventilation cases and passive cases
 - Both consist of 1 m³ TCS geometry
 - Active ventilation includes chimney extract
 - Passive ventilation includes ambient domain and passive vents
- Mesh refinement cones around H₂ jet release and active ventilation
- H₂ inlet taken as expanded diameter from pseudo source



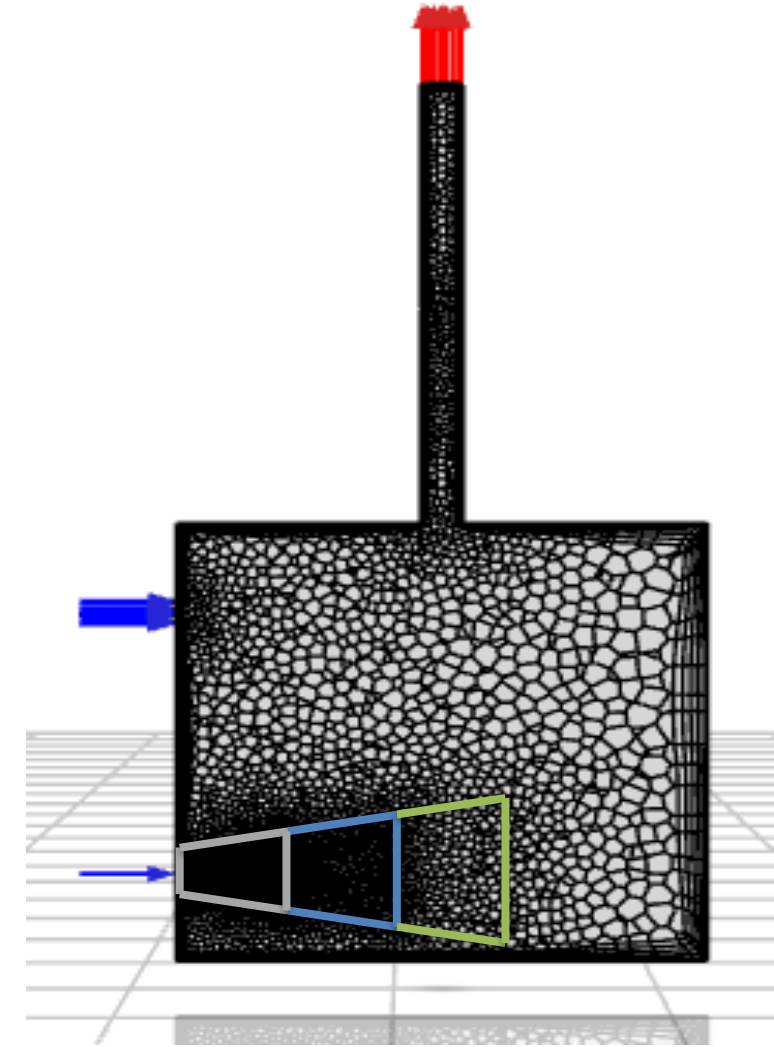
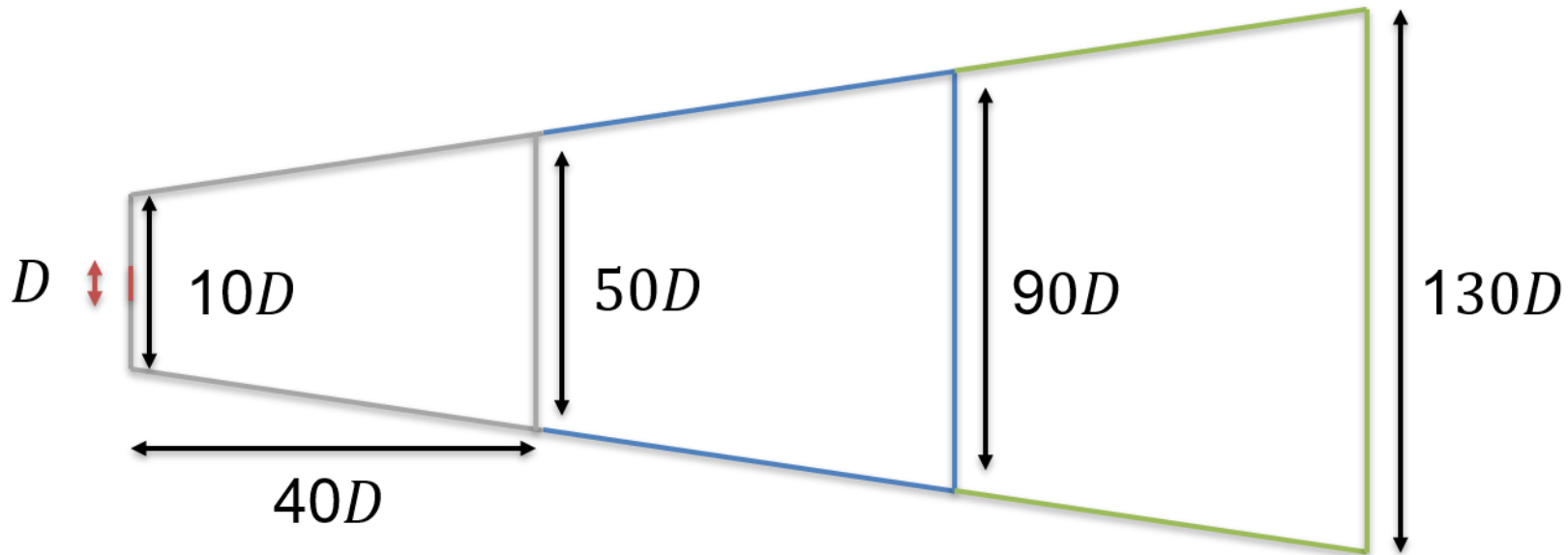
Geometry for active ventilation cases



Geometry for passive ventilation cases

Meshes

- Meshing strategy based on expanded nozzle diameter (D), to balance simulation time and accuracy
- Polyhedral cell type used



Example polyhedral medium mesh

Meshes

	Inlet cell sizing	Zone 1	Zone 2	Zone 3	Max size
Coarse	D/2.5	4D	8D	16D	128 mm
Medium	D/5	2D	4D	8D	64 mm
Fine	D/10	1D	2D	4D	32 mm

Table: Mesh refinement zone sizing based on nozzle diameter

Physics setup – Active cases

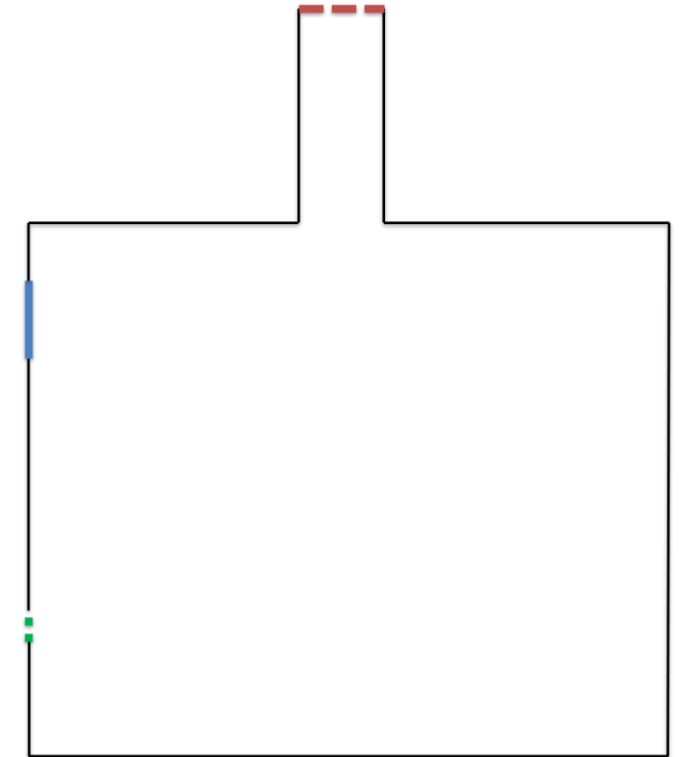
- H2 release (mass flow rate)
 - Pseudo source approach
 - Phast predicted, mass flow, expanded diameter and temperature
- Walls
 - Adiabatic, no slip.
- Active ventilation flow (mass flow rate)
 - Convert volumetric flow rate L/min to kg/s

$$\dot{m}_{air} = \frac{Q_{air}}{60 \times 10^3} \rho_{air}$$

- Species mole fractions fractions, based on relative humidity (RH) and ambient temperature (T_{amb})

$$\phi_{H_2O} = \frac{SVP_{H_2O}(T_{amb}) \times RH}{P_{atm}}, \quad \phi_{O_2} = 0.21,$$

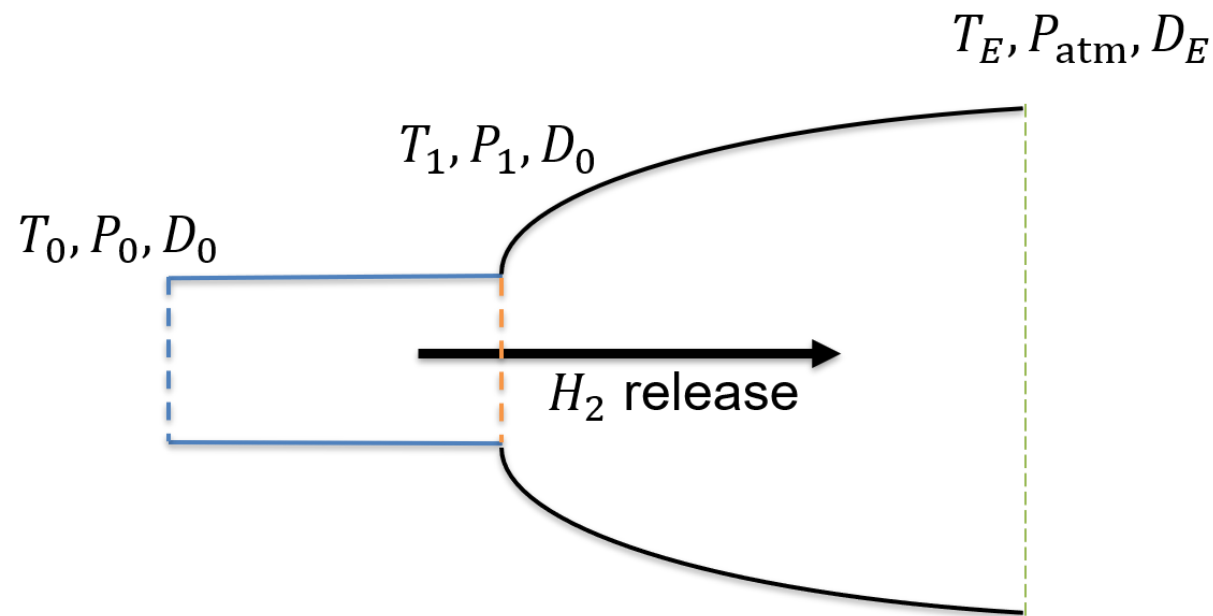
$$\phi_{N_2} = 1 - \phi_{H_2O} - \phi_{O_2}$$



- Active Ventilation inlet
- ... H2 inlet
- Walls
- - - Pressure outlet

Modelling problem description

Take the steady nozzle pressure and nozzle temperature as storage conditions for release through the orifice. Modelled the mass flow rate using both Phast V9 and using the choked flow equation.



$$\dot{m} = C_d A \sqrt{\gamma \rho_0 P_0 \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}}}$$

Experimental Steady Orifice Conditions				Phast				Choked flow using T_0, P_0
Test #	T_0 (K)	P_0 (barg)	D_0 (mm)	T_1 (K)	T_E (K)	D_E (mm)	$\dot{m}$ (g/s)	$\dot{m}$ (g/s)
3	262.05	1.40	0.20	216.87	203.13	0.18	0.0039	0.0042
4	209.78	5.62	0.20	173.01	127.14	0.24	0.0130	0.0131
5	182.73	5.00	0.20	150.45	112.52	0.23	0.0126	0.0128
6	153.49	7.64	0.50	126.20	88.64	0.66	0.1251	0.1265
7	115.86	6.84	0.50	95.18	67.78	0.63	0.1306	0.1345
8	186.15	2.76	0.50	153.32	127.10	0.50	0.0478	0.0496
9	183.52	4.44	0.50	151.13	115.23	0.56	0.0711	0.0723
10	150.03	1.88	1.00	123.42	109.75	0.93	0.1593	0.1710
11	127.08	1.75	1.00	104.45	94.08	0.92	0.1644	0.1790
12	117.47	2.26	1.00	96.61	83.05	0.96	0.2066	0.2220
13	90.96	2.09	1.00	74.75	65.18	0.94	0.2217	0.1995
14	90.93	6.97	1.00	74.58	52.86	1.27	0.6015	0.3896
15	52.62	6.05	1.00	42.98	30.84	1.22	0.7116	0.7715
16	33.62	7.63	1.80	27.84	20.39	2.61	4.1738	4.8561
17	34.13	7.81	1.80	28.24	20.39	2.60	4.1496	4.8715
18	44.85	2.91	1.80	36.75	30.04	1.81	1.3450	1.4915
19	63.01	1.61	1.80	51.73	47.28	1.63	0.7162	0.8111
20	68.21	2.27	1.80	55.99	48.06	1.72	0.8856	0.9759
21	34.26	6.87	1.80	28.31	20.39	2.43	3.5955	4.1372
22	161.13	1.82	1.00	132.60	118.61	0.92	0.1501	0.1607
23	103.20	7.60	1.00	84.69	59.38	1.31	0.6091	0.6311
24	174.62	8.06	0.50	143.67	100.28	0.67	0.1230	0.1236
25	204.15	7.63	0.20	168.22	118.36	0.26	0.0173	0.0173
26	220.55	2.83	0.20	181.99	150.27	0.20	0.0072	0.0064

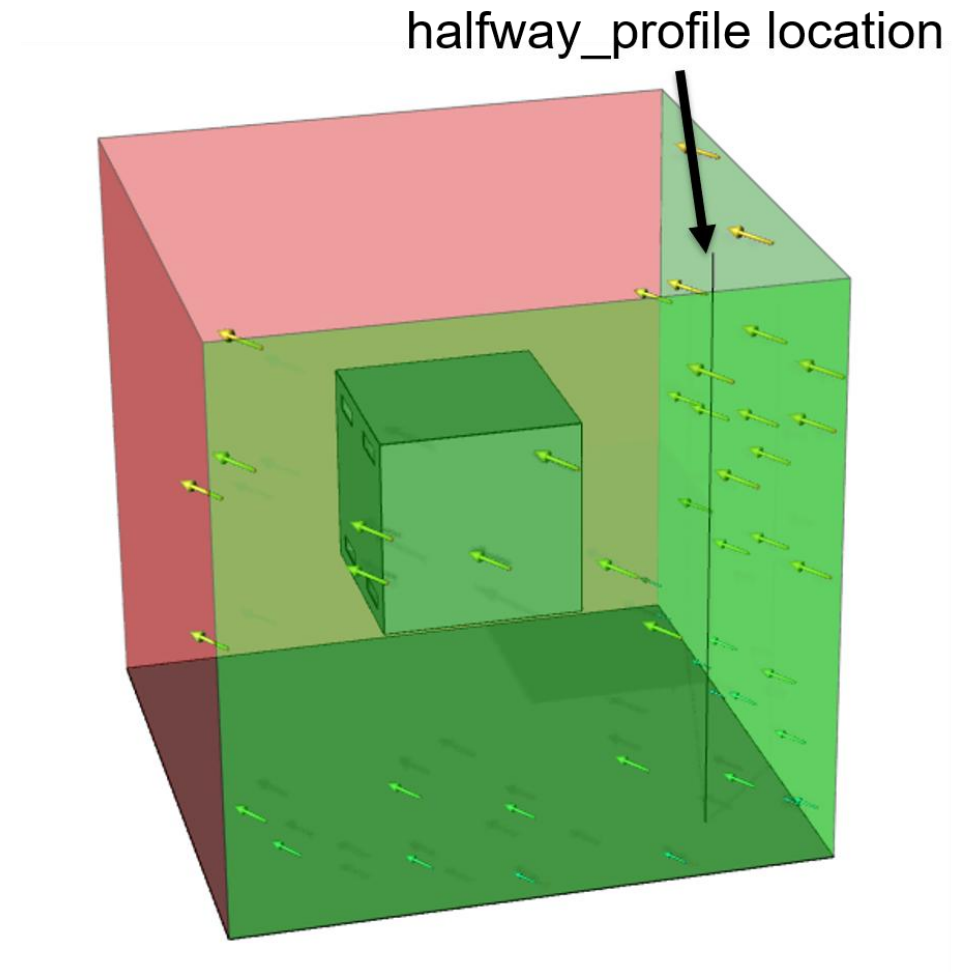
Wind profile

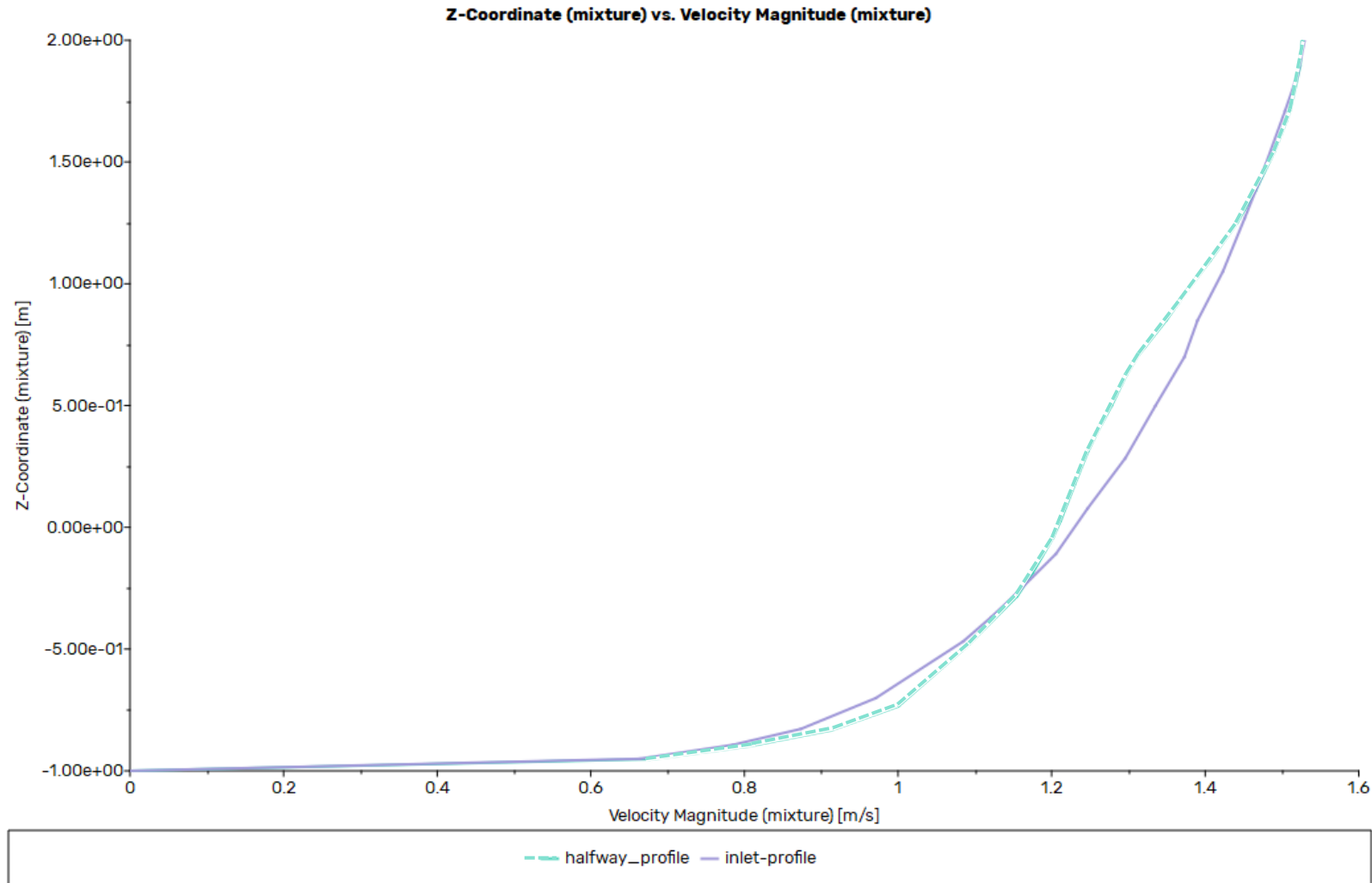
Assumed a power law profile

- $U_{\text{mag}} = U_m K z^a$
- $K = 0.52$ and $a = 0.2$

Passive ventilation domain

- ambient inlets (green) on the front and right face
- outlets (red) on the left, back and top face
- Wall on the bottom face





Wind profile at the inlet face (purple) and along a profile further into the domain (blue)

Other physics setup – Slide 1

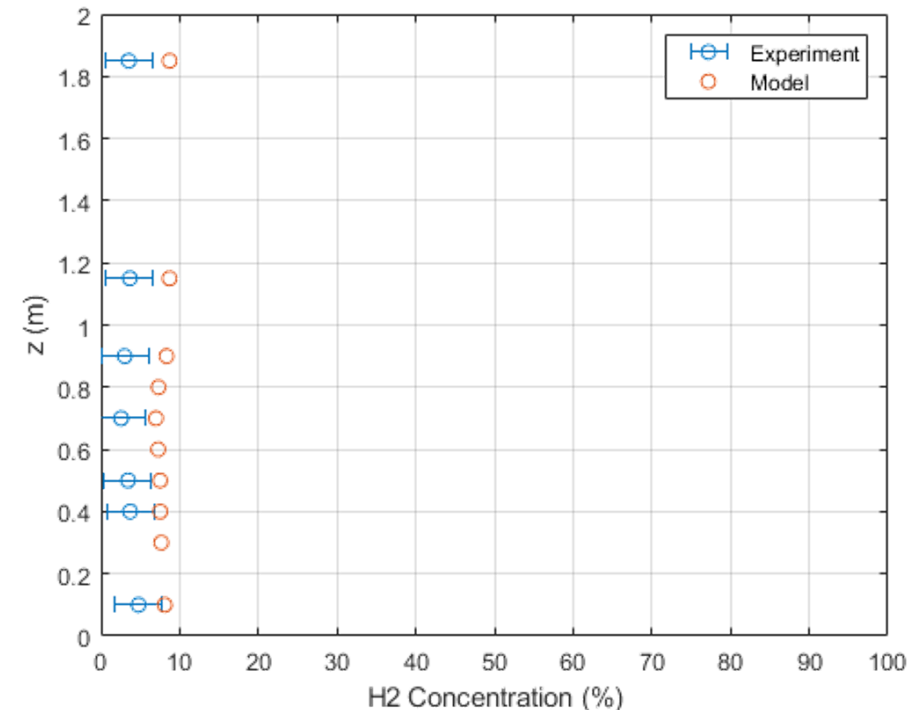
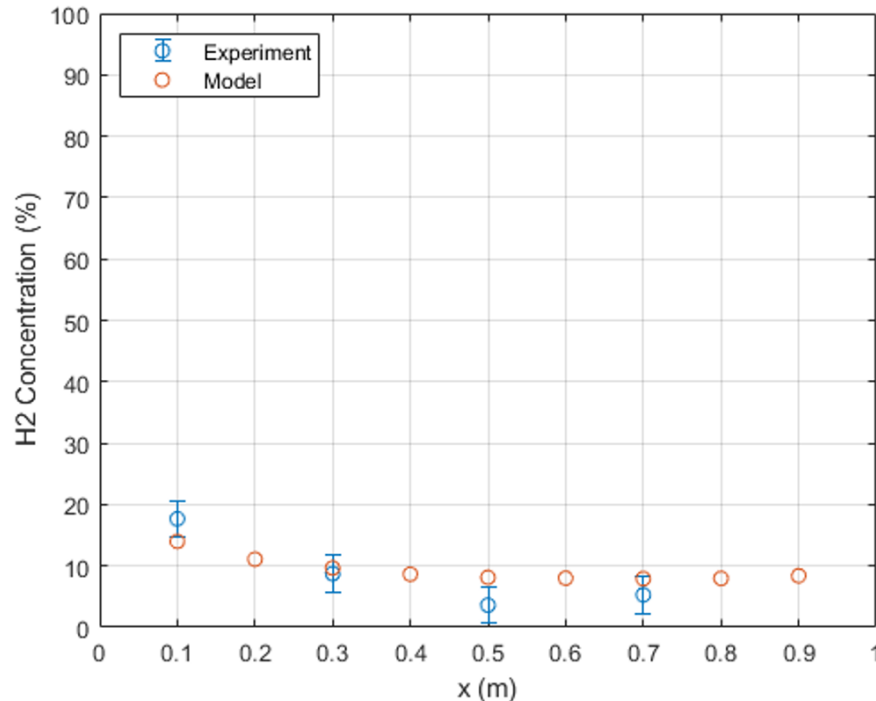
- The CFD software Ansys Fluent V24 R2 was used to simulate these cases.
- Simulated the release in two stages
 - **Phase 1**: Model cold H₂ jet without phase change to develop temperature, pressure and velocity fields
 - **Phase 2**: Enable mass transfer between the gaseous and liquid phases to quasi-steady state
- Turbulence model
 - $k - \omega$ SST model
- PV algorithm
 - Coupled algorithm, global time step pseudo time stepping method
 - Time scale factor of 0.3

Other physics setup – Slide 2

- Mixture model
 - 4 Phases (Gas mixture, Liquid O₂, Liquid H₂, Liquid N₂)
 - Ideal gas assumption
- Mass transfer
 - Modified Lee model for evaporation/condensation of substances
 - Initial Lee model relaxation coefficients of 0.1 s⁻¹ for H₂, N₂ and O₂. H₂O was neglected due to solution stability
 - Literature showed a range of values. It was noted that the Lee model is inherently sensitive to mesh, time step, physics setup and should be tuned for the specific problem and setup

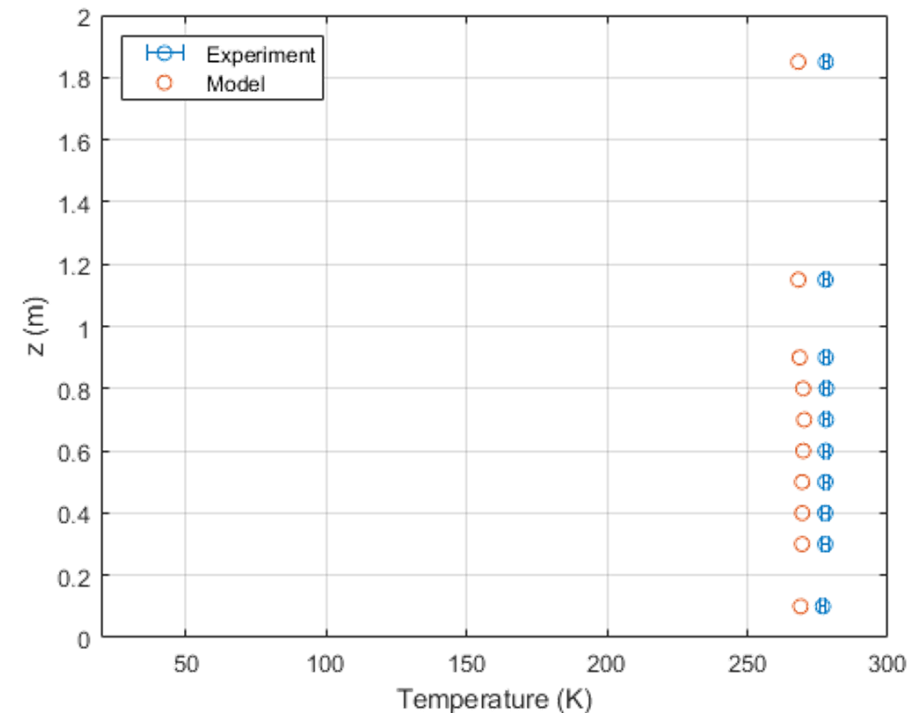
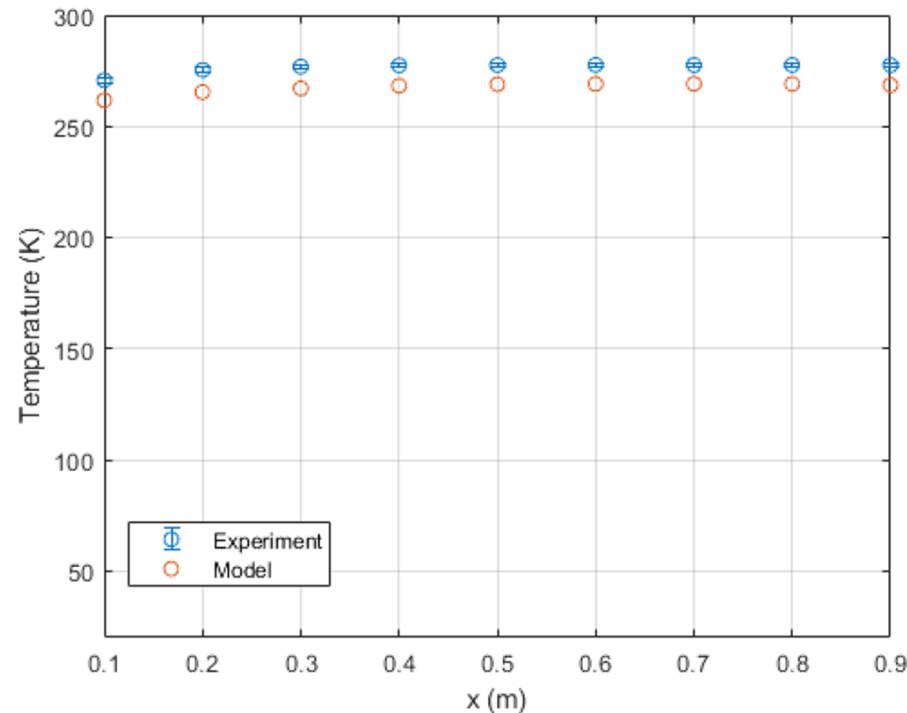
Experimental comparison – Active ventilation, Test 8

- Relatively good agreement can be seen for concentration predictions
- Overpredictions in hydrogen concentration points to possible mass flow overprediction



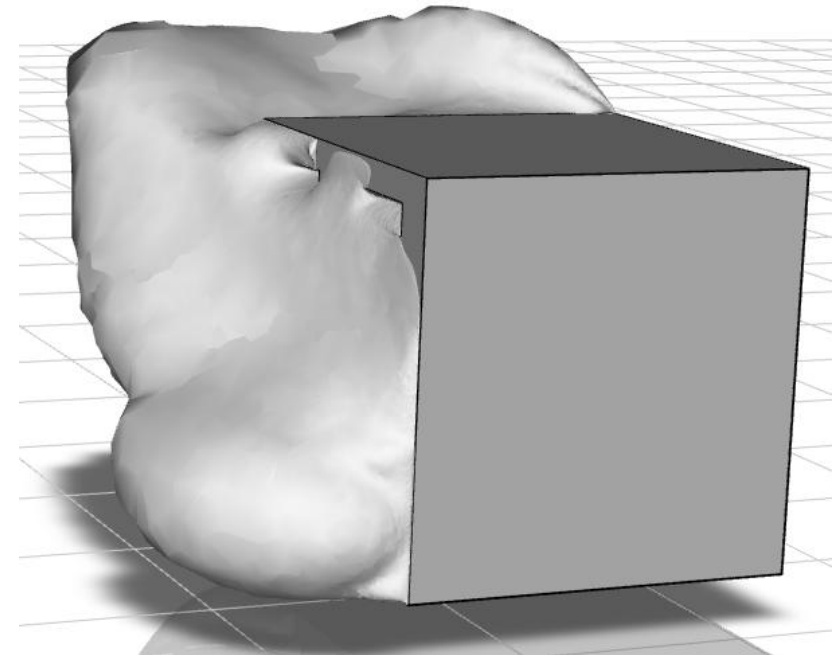
Experimental comparison – Active ventilation, Test 8

- Temperature predictions were 10 K colder than experimental measures.
- Not accounting for condensation of the ambient water vapour or additional heat source from the TCS wall conduction.



Qualitative Comparison – Passive dispersion, Test 21

- External H_2 passive dispersion
 - Plot of isosurface H_2 mole fraction = 4%
 - Captures release from TCS and directional external dispersion aligned with flow field
 - Only a snapshot. Passive cases inherently an unsteady flow problem as seen experimentally



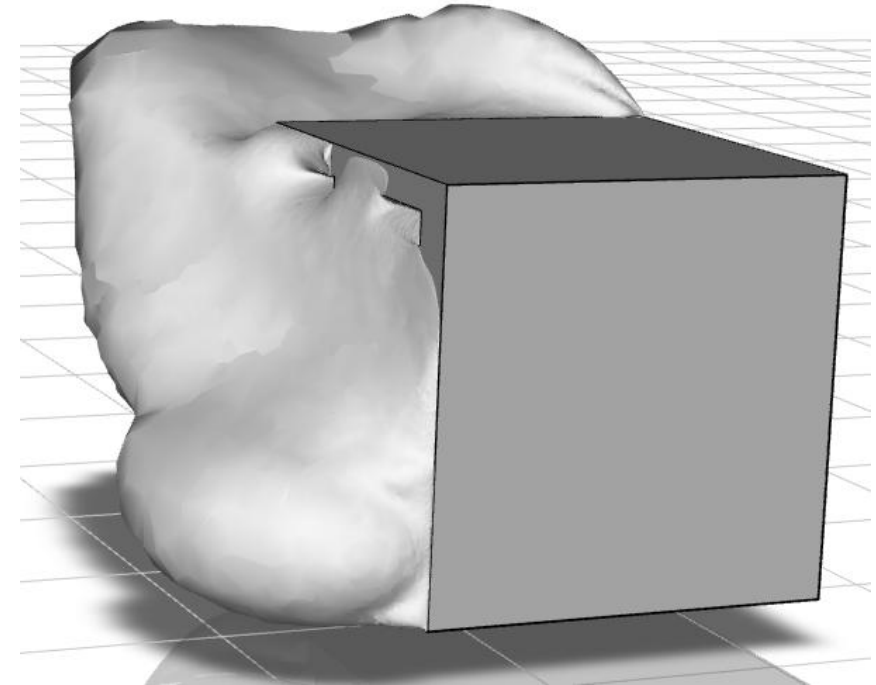
Isosurface for H_2 mole fraction of 4% showing air inflow in the top vents and exhaust through bottom vents.

Qualitative Comparison – Passive dispersion

Test 21



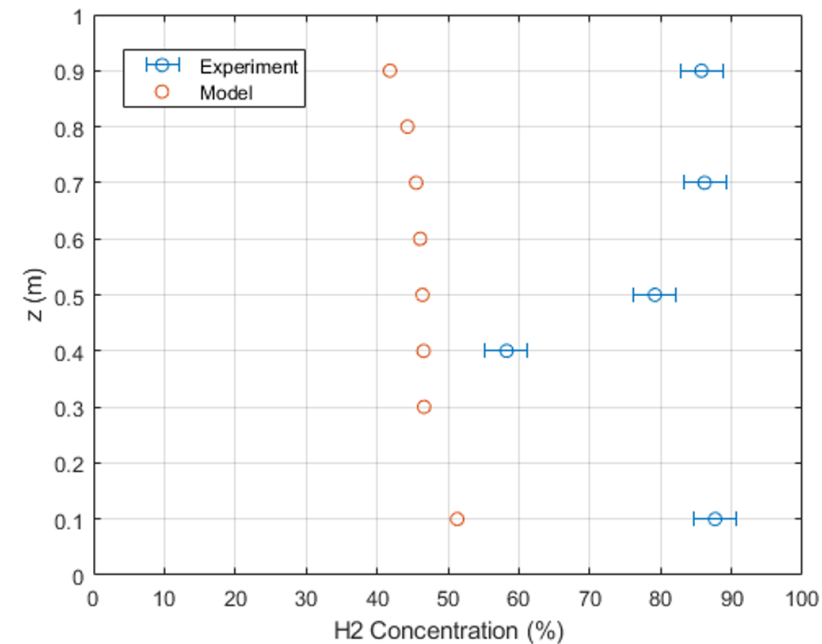
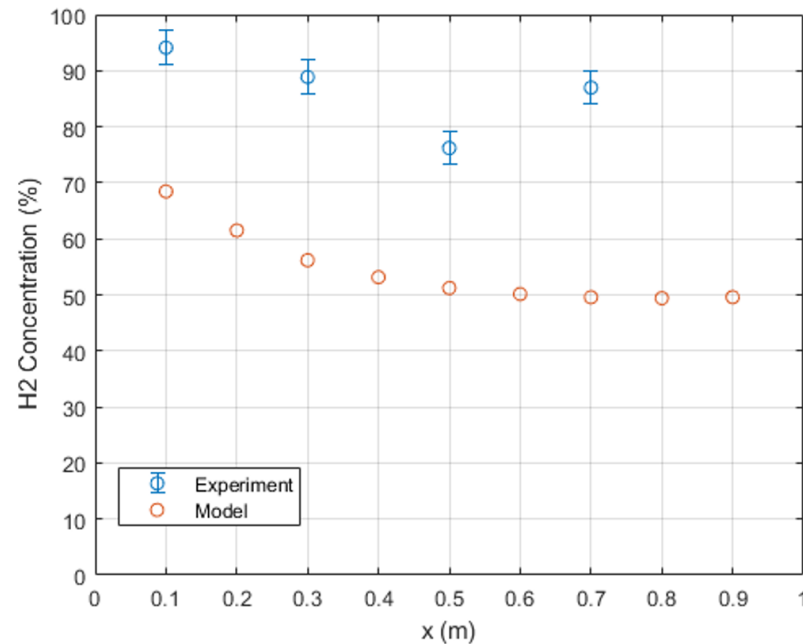
Image taken from an experimental passive release test video



Isosurface for H_2 mole fraction of 4% showing air inflow in the top vents and exhaust through bottom vents.

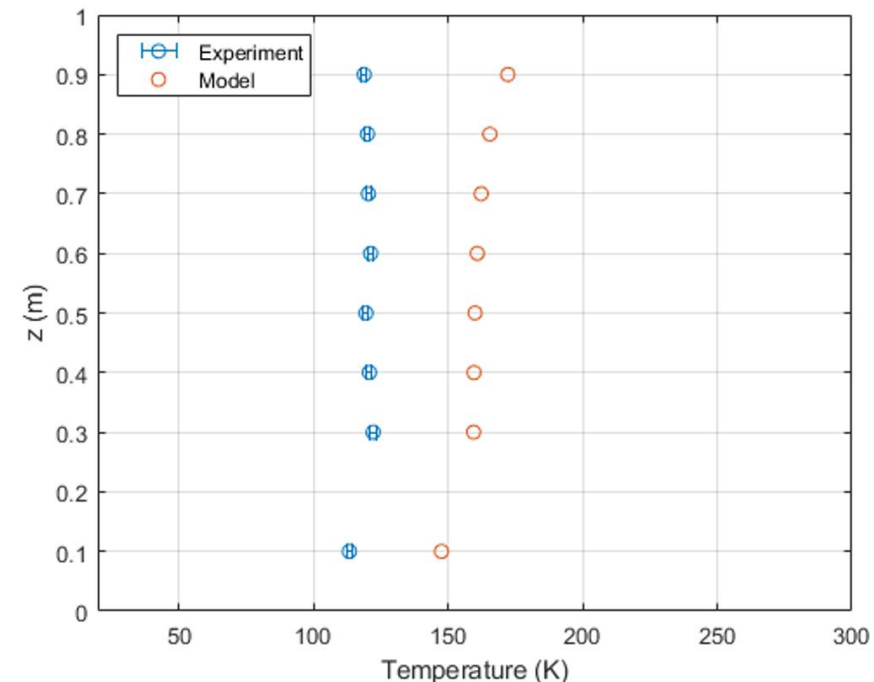
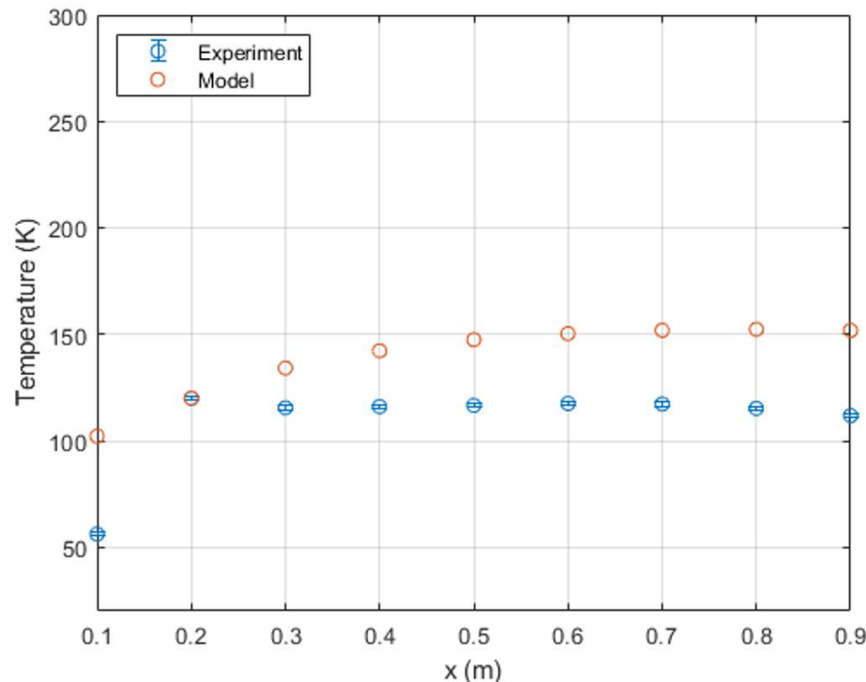
Experimental comparison – Passive ventilation, Test 21

- The model considerably underpredicted the hydrogen concentration
- Possibly over dilution due to the ambient flow or underprediction of the mass flow rate and phase quality.

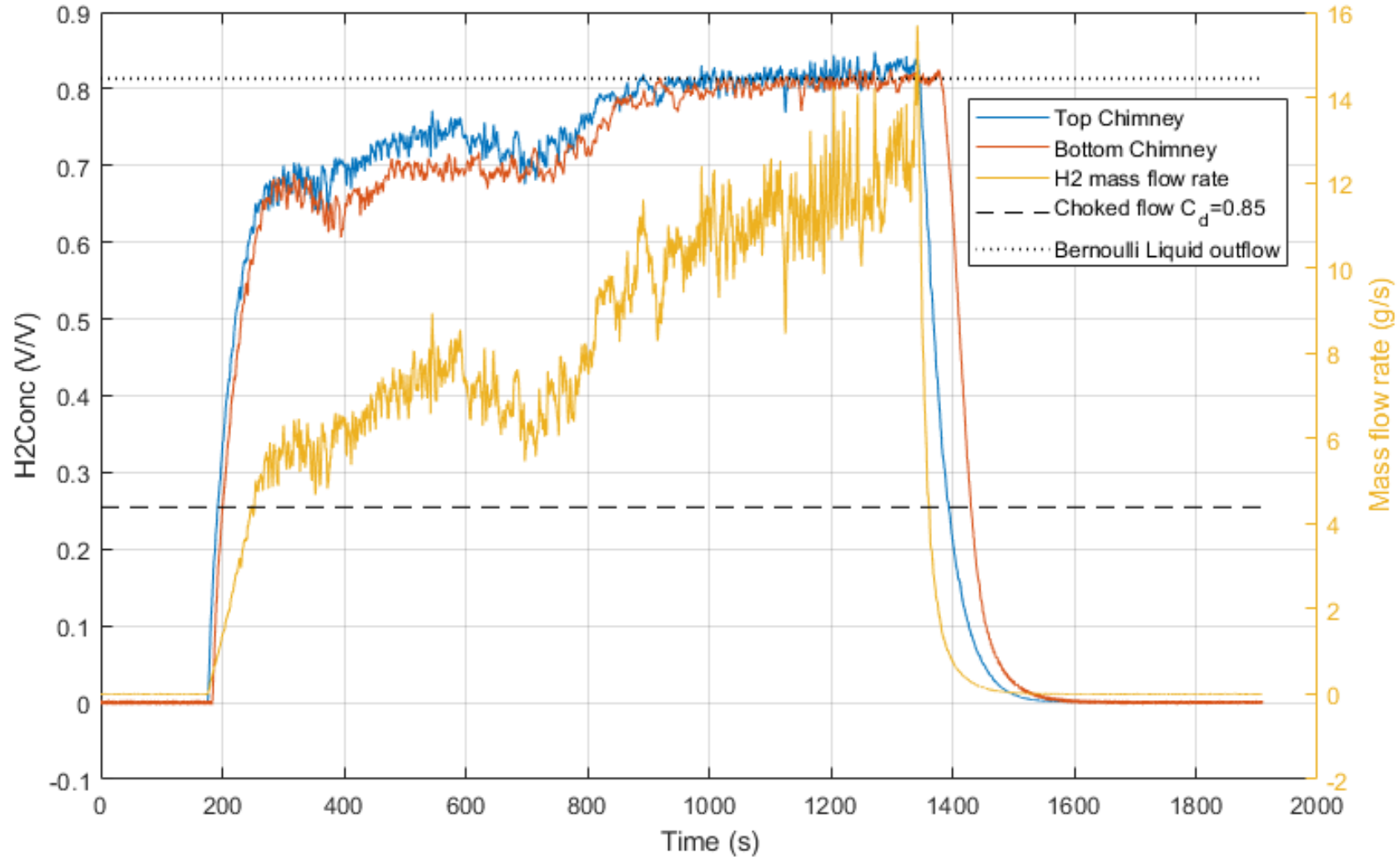


Experimental comparison – Passive ventilation, Test 21

- The model also overpredicted the temperature.
- Again, possibly over dilution due to the warmer ambient flow or underprediction of the mass flow rate and phase quality.



Example: Test 17 (8 barg, 1.8 mm, Active)



Left axis - Hydrogen volume concentration at the bottom (orange) and top (blue) of the chimney

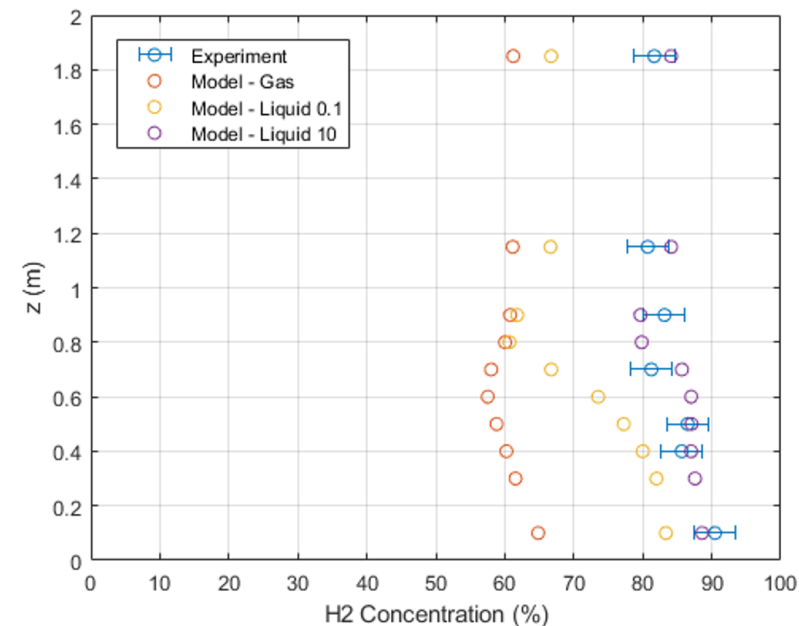
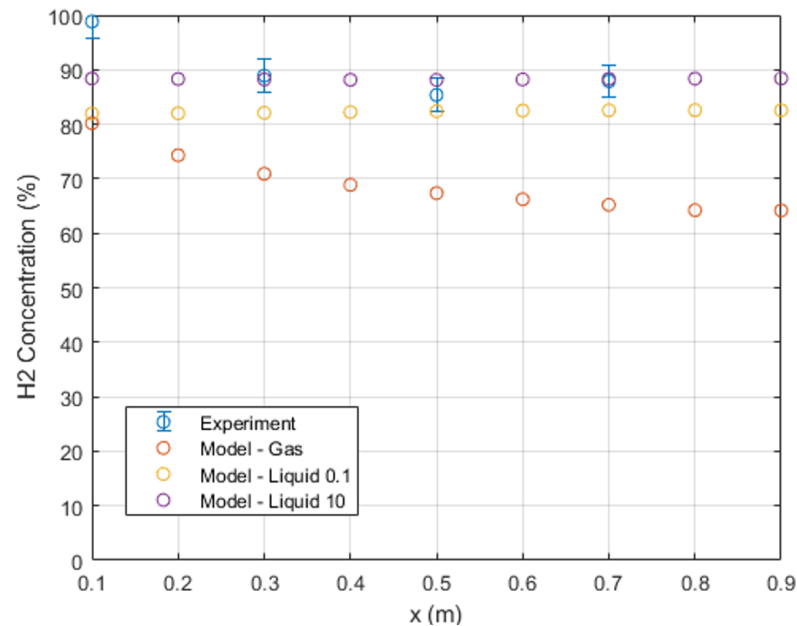
Right axis - Back calculated mass flow prediction (Yellow) with choked flow (black dashed) and Bernoulli outflow (black dotted)

Example: Test 17 (8 barg, 1.8 mm, Active)

- Mass flow predicted to change throughout the test
- Phast gaseous flow predicted 4.14 g/s
- Transition from choked flow prediction to liquid outflow
- Unknown interesting phenomena occurring at approximately 800 s.

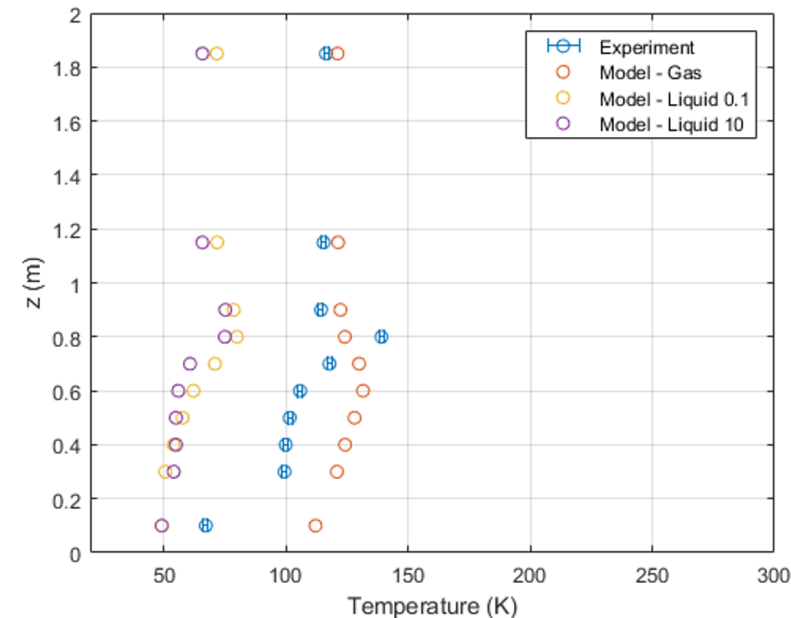
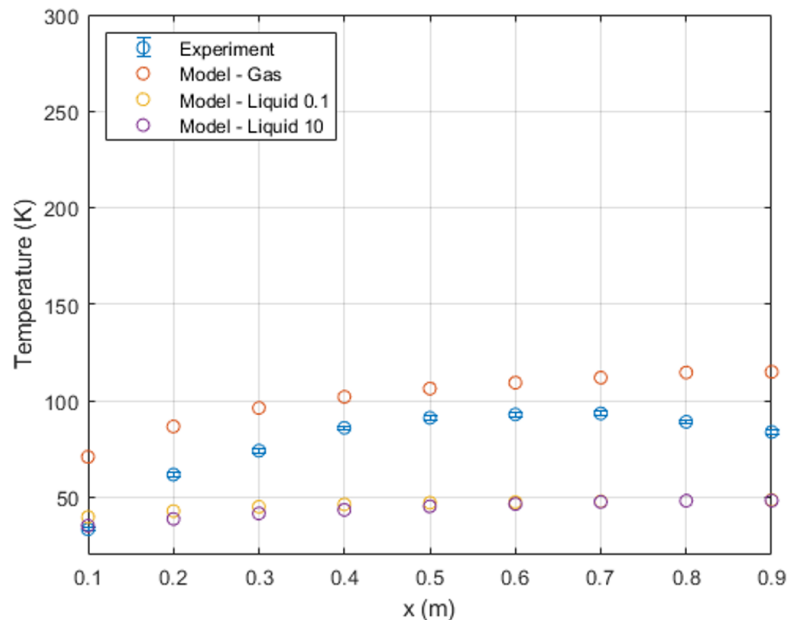
Experimental Comparison – Active ventilation, Test 17

- Using a choked release (gas) underpredicts the concentration
- A liquid release with a varying Lee coefficient can achieve good predictions for concentration.



Experimental Comparison – Active ventilation, Test 17

- Using a choked release (gas) overpredicts temperature. A liquid release with a varying Lee coefficient will considerably underpredicts temperature.
- This suggests that a two-phase release may be most appropriate with further tuned coefficient.



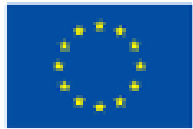
Conclusions

- A pseudo-steady 3D numerical model has been developed for predicting liquid hydrogen leaks into an enclosure.
- The model provides insight into the internal dispersion dynamics within the enclosure and provides indicative H₂ concentrations that may build up within the enclosure
- For cases where significant warming has occurred in the pipework the model provides reasonable predictions.
- For cases where potential two-phase releases are present the model shows sensitivity to the Lee model coefficients.
- Further development of the model is needed before reliably using the model to predict the potential hazards from the enclosure.

Further work

- Initial model still requires further development. Potential areas:
 - Influence of alternative equations of state (EoS), currently uses ideal gas but could couple a more advanced EoS e.g. PR, Helmholtz.
 - Simulating the cases using a transient modelling approach. Ambient wind field is inherently transient. The solution currently takes steady state conditions, however, the release dynamics are transient, taking time to reach these steady conditions.
 - Current results suggest that for large pressure and nozzle sizes a two-phase release is present. Incorporation of a two-phase release should be included and comparison of its impact on the dispersion dynamics in the TCS.
 - Tuning of the Lee model coefficients but also investigating alternative modelling approaches for phase transfer.

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Thank you for your attention

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