A MULTI-STAGE MODELING APPROACH FOR RAINOUT, POOL FORMATION, AND DISPERSION OF LIQUID HYDROGEN RELEASES

6th ELVHYS online workshop – Project achievements, remaining knowledge gaps and technological bottlenecks

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Introduction and Motivation

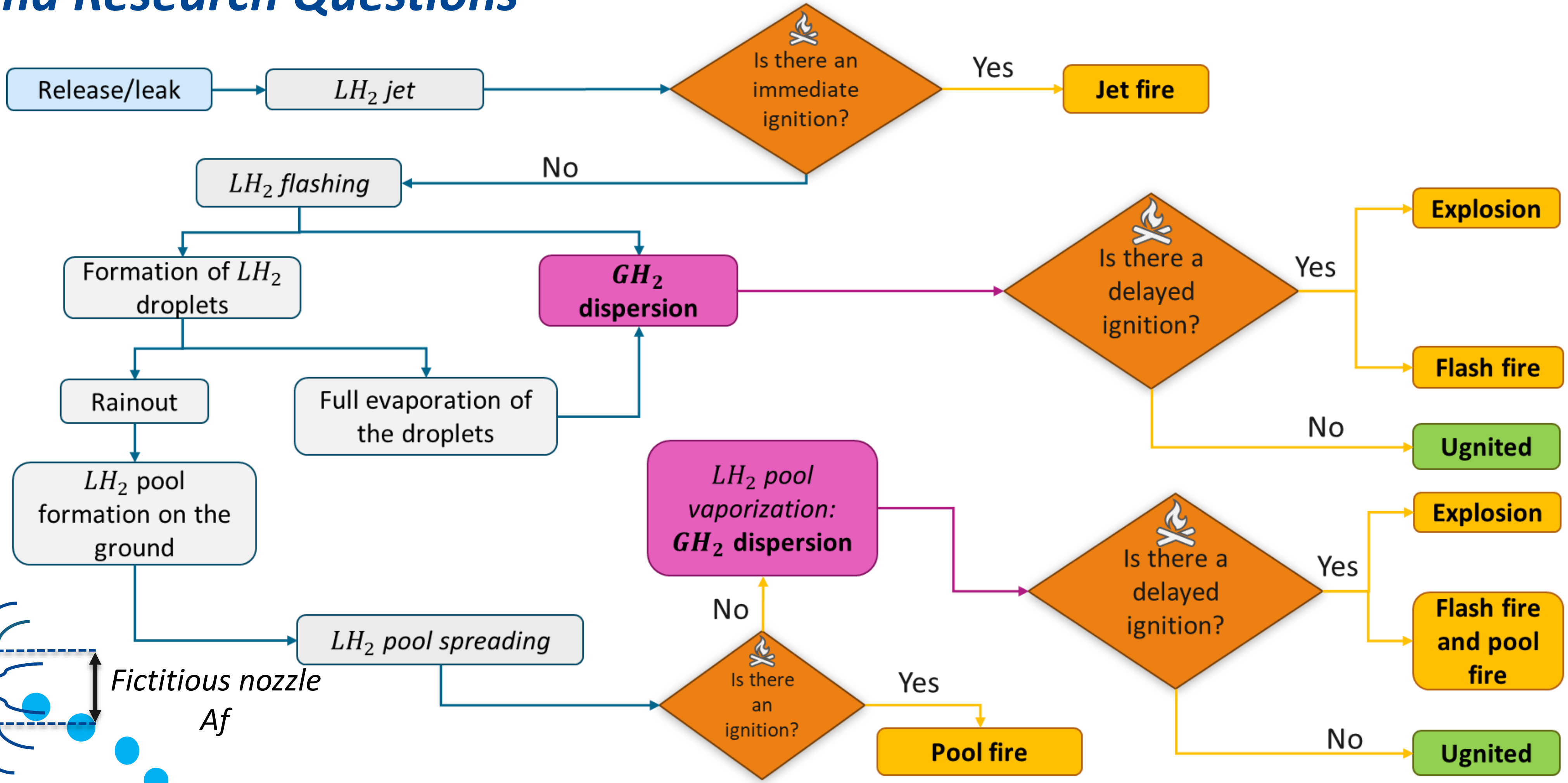
Why do we need **Liquid *Hydrogen* (LH_2)**?

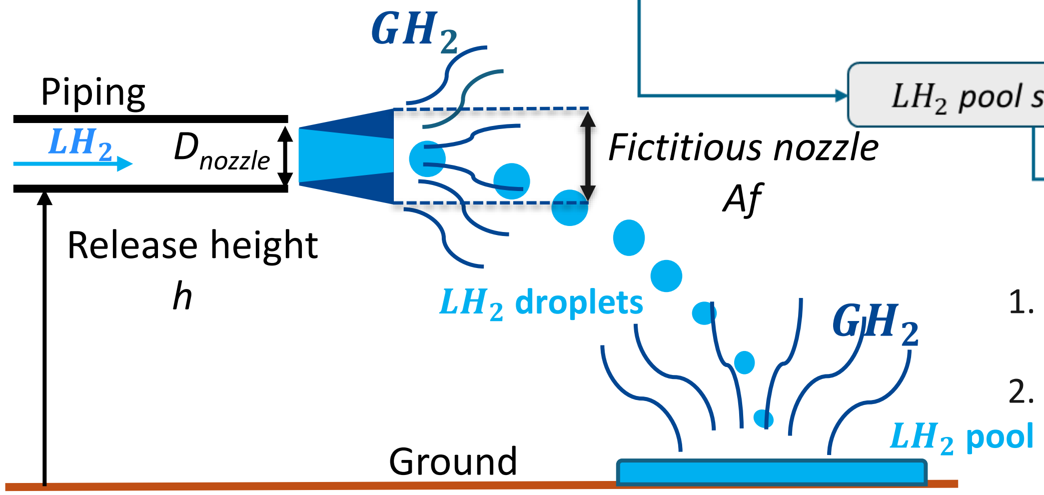
- **High energy density per unit mass** (120 MJ/kg)
- **Carbon-neutral fuel**
- It can be **used** for **many applications**

What are the **Safety Issues** related to the **use** of **LH_2**?

- **High flammability**
- **Severe consequences from Loss of Containment**
- **Stored at cryogenic temperatures** from 13.6 K to 33.15 K

Safety Issues and Research Questions





1. How can the **release** of LH_2 be **simulated**?
2. How can the **droplet size** of LH_2 be **calculated**?
3. How can the **rainout** of LH_2 be **quantified**?
4. How can the **pool** of LH_2 be **estimated**?
5. How can the **dispersion** of GH_2 be **simulated**?

Methodology: why " MULTI-STAGE MODELING APPROACH"?

Input for DISCHA:
- Pipe design parameters (diameter, length, thermal conductivity, etc.)
- Pressure after the release valve
- Saturation temperature
- Nozzle diameter
- Vapor quality within the pipe after the release valve

DISCHA [1]
1° step

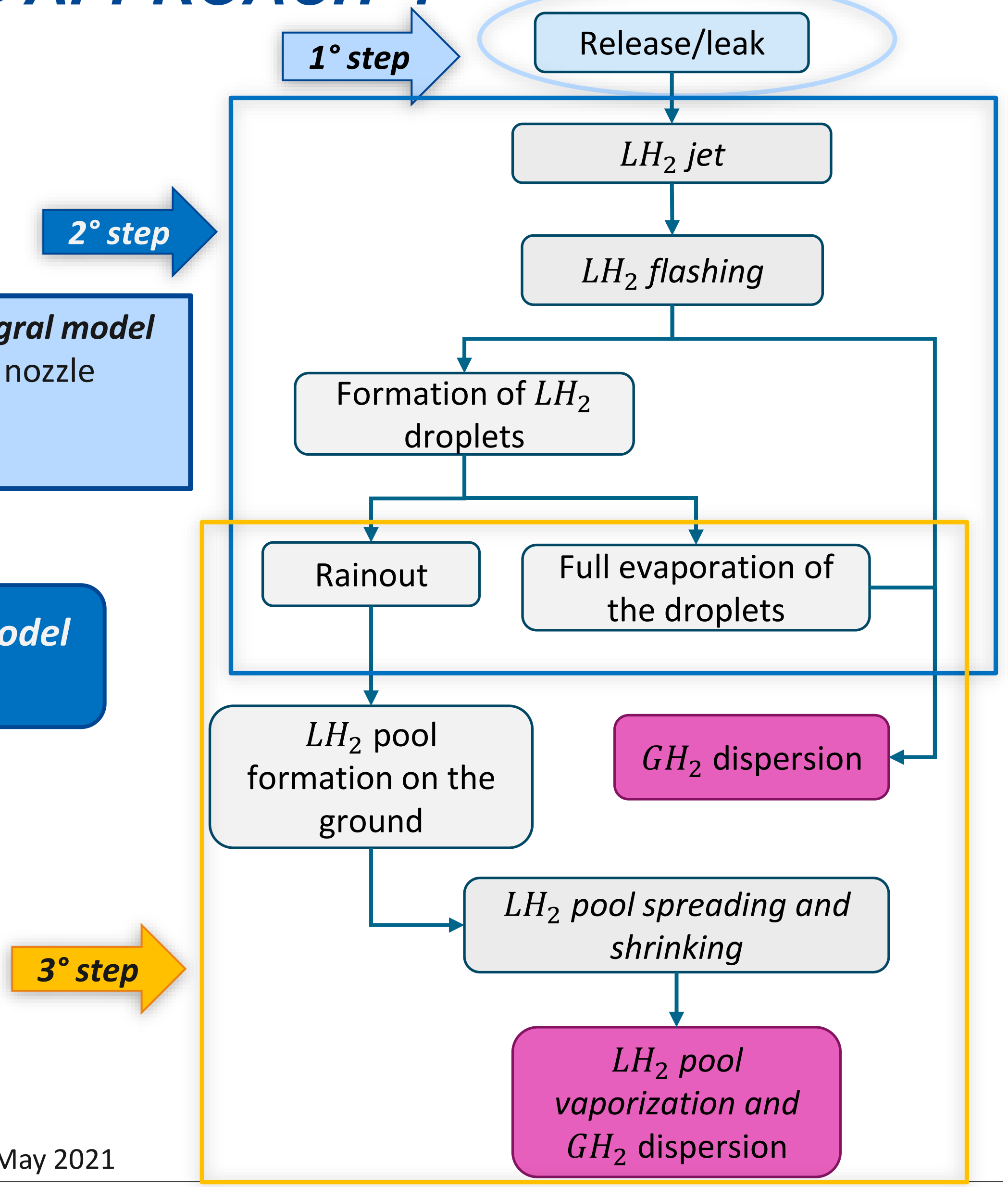
Output of DISCHA/Input for the integral model
- Pressure and temperature at the nozzle
- Vapor quality at the nozzle
- Velocity at the nozzle

Integral Model
2°step

Output of the IM/Input for the CFD
- Jet velocity at the fictitious nozzle
- Vapor quality at the fictitious nozzle
- Droplet diameter
- Droplet evaporation
- Rainout on the ground

CFD (KFX)
3°step

Output of the «Multi-Stage Approach»
- Droplet evaporation
- Rainout on the ground
- Pool formation and spreading
- Pool vaporization
- GH_2 dispersion



[1] Venetsanos A.G., An engineering tool for discharge calculations, PRESLHY dissemination conference, May 2021

Methodology: 1 ° and 2° Steps

2.1° Step:
Calculation of the fluid quality after flashing:

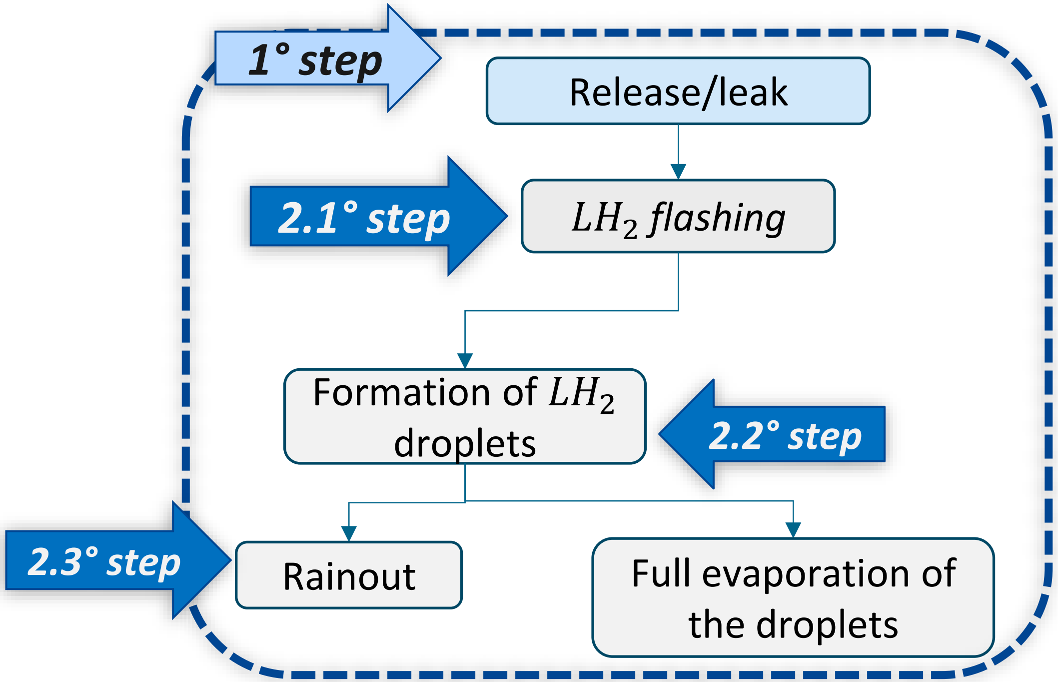
- $\phi_{m,f} = 1 - \frac{H_{vf} - H_{ve} + (1 - \Phi_e)\cdot L_{ve} + 0.5 \cdot \left(u_f^2 - u_e^2\right)}{L_{vf}}$

2.2° Step:
Calculation of the droplet size after flashing with mechanical break-up criteria:

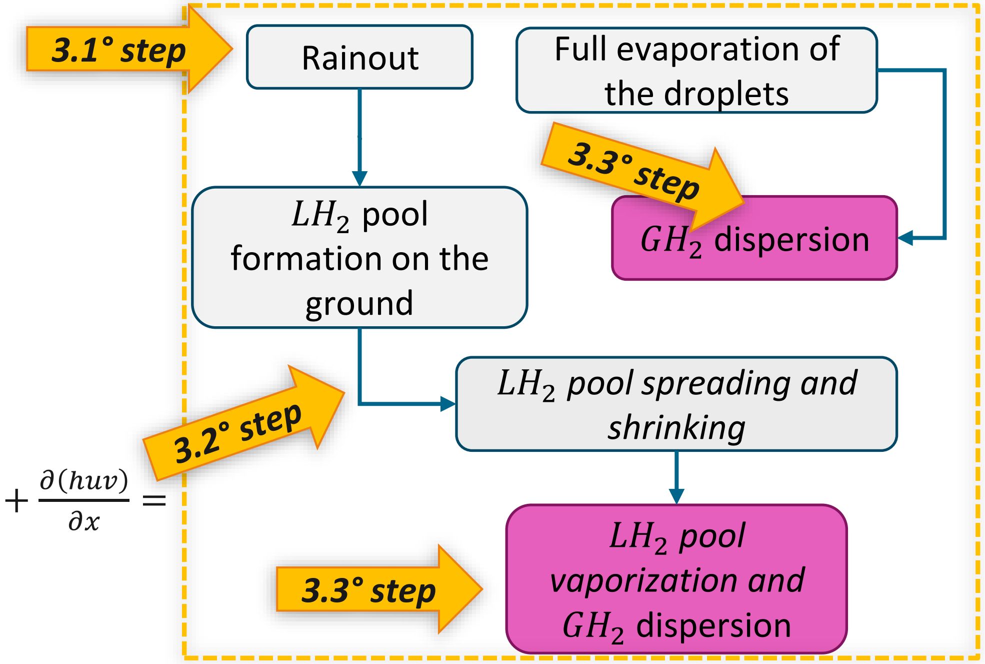
- $d_{d,f} = C_{ds} \cdot \frac{\sigma_s}{{u_f}^2 \cdot \rho_a}$

2.3° Step:
Calculation of the droplet evaporation and <u>rainout</u> on the ground:

- Droplet evaporation constant: $k_B = \frac{4 \cdot \mu_i \cdot D \cdot P_a}{\rho_{Lf} \cdot R \cdot T_a} \cdot ln\left(1 + \frac{P_s(T_d)}{P_a}\right)$
- Droplet evaporation rate: $\frac{d}{dt} d_d = -\frac{k_B}{d_d} \cdot \left(1 + 0.28 \cdot {Re_d}^{\frac{1}{2}} \cdot {S_c}^{\frac{1}{3}}\right)$
- Net vapor mass released by the jet: $q_V = q_{S,e} \cdot \phi_{m,f} + (1 - \phi_{m,f}) \cdot \left(1 - \left[\frac{d_0}{d_d}\right]^3\right) \cdot q_{S,e}$
- **Rainout**: $q_L = q_{S,e} - q_V$



Methodology: 3° Step with CFD (KFX)



3.1° Step:

Lagrangian approach for droplet tracking

3.2° Step:

Pool Spreading: KFX uses an SHW model to simulate the spreading behavior:

- Continuity eq.: $\frac{\partial h}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (hv)}{\partial y} = -\dot{m}_{evap}$
- Momentum eq.: $\frac{\partial (hu)}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2} g h^2\right) + \frac{\partial (huv)}{\partial y} = -\tau_x \; \frac{\partial (hv)}{\partial t} + \frac{\partial}{\partial y}\left(hv^2 + \frac{1}{2} g h^2\right) + \frac{\partial (huv)}{\partial x} = -\tau_y$

Net Heat transfer between the cryogenic pool and the ground:

- $q_{\text{ground}} = -k \left.\frac{\partial T}{\partial z}\right|_{z=0} = \alpha \rho c_p \left.\frac{\partial T}{\partial z}\right|_{z=0}$

3.3° Step:

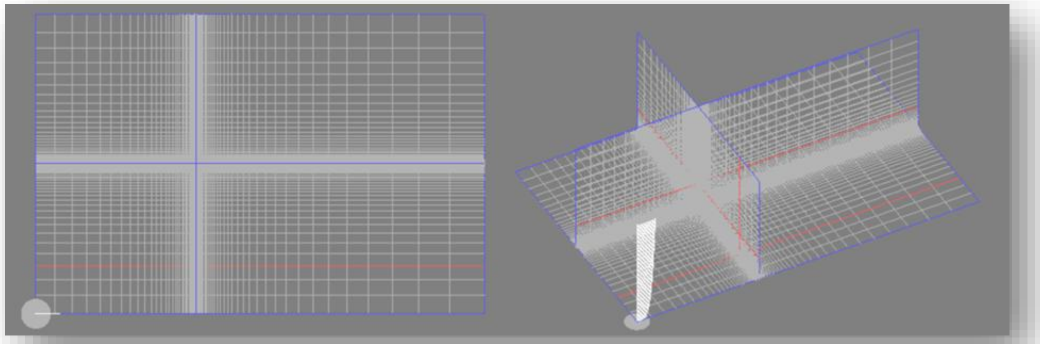
Gas dispersion with Reynolds-Averaged Navier-Stokes (RANS) equations:

Continuity eq.: $\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho}\tilde{u}_j)}{\partial x_j} = \bar{\rho}\tilde{R}_{liq}$

Momentum eq.: $\frac{\partial (\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial (\bar{\rho}\tilde{u}_j\tilde{u}_i)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\tau_{ij} - \bar{\rho}\tilde{u}_j^{"}u_i^{"}\right) + \bar{\rho} f_i + \bar{\rho}\tilde{F}_{liq,i}$

Energy eq.: $\frac{\partial (\bar{\rho}\tilde{h})}{\partial t} + \frac{\partial (\bar{\rho}\tilde{u}_j\tilde{h})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(k \frac{\partial \tilde{T}}{\partial x_j} - \rho \sum_l Y_l V_{lj} h_l - \rho u_j'' h''\right) + \bar{Q}_{gs} + \bar{Q}_{Rad} + \bar{\rho}\tilde{S}_{liq}$

Computational grid configuration used in the simulation



- 733,642 nodes were used by configuring 139, 91, and 58 nodes in the x-, y-, and z-directions
- The grid size at the release point was 0.0482 m,

Methodology: Case Study

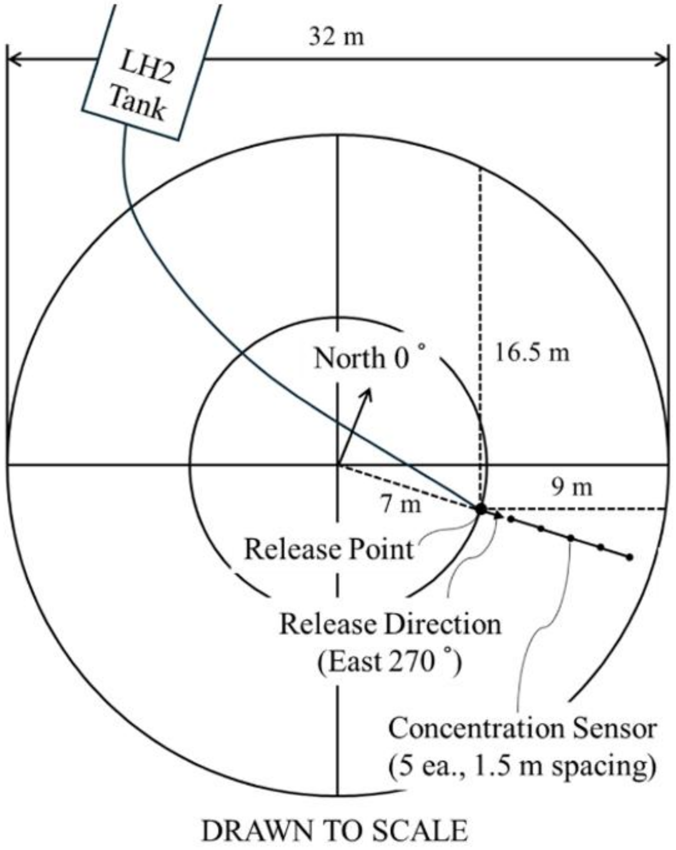
Simulations were carried out and compared with the **experimental data** from **Test 5** and **Test 7** of the Health and Safety Executive **(HSE) experiments** [2]

Parameter	Test 5	Test 7
Nominal release pressure	1.2 bar	1.2 bar
Release rate	0.070 kg/s	0.070 kg/s
Delivery pipe diameter	25.4 mm	25.4 mm
Relesease height	Ground level	0.86 m
Wind speed and direction	2.7 m/s, 270°	2.9 m/s, 297°
Fluid quality at the nozzle	Unkown	Unkown

[2] M. Royle and D. Willoughby, "Releases of unignited liquid hydrogen," Health and Safety Laboratory Report No. RR986, Health and Safety Executive (HSE), United Kingdom, 2014.

Test 5: Horizontal ground release [2]

Test 7: Horizontal release from a height of 0.86 m [2]



LH_2 **spill test layout** and geometries used in KFX (adapted from [2])

- The **gas concentration sensors** are mounted on **five vertical rods**. The rods are positioned at **distances** of 1.5 m, 3.0 m, 4.5 m, 6.0 m, and 7.5 m from the leak point. On each rod, the sensors are placed **at heights** of 0.25 m

Results: LH_2 Rainout

For **Test 7**, the **integral model confirmed** that **no rainout occurred** under the **experimental setup conditions:** the **LH_2 droplets evaporate** before reaching the **ground.** Causes [3]:

- The **higher** the release **height**, the **lower** the **rainout,** but
- The thermodynamic conditions of LH_2 led to high **jet velocity**: the **higher** the **jet velocity**, the lower the **rainout**
- The **higher** the **pressure** at the nozzle, the **lower** the **rainout**
- The **higher** the **vapor quality** at the nozzle, the **lower** the **rainout**

For **Test 5**, the **CFD** and **integral model** showed **good agreement**, with a rainout rate difference of only **0.6%**

Jet velocity	*Fictious nozzle diameter*	*Droplet diameter after flashing*	*Liquid fraction after flashing*	*Rainout on the ground*
3.29 m/s	25.289 mm	2.126 mm	0.987 (-)	0.069 kg/s

Test 7: Horizontal release from a height of 0.86 m [2]

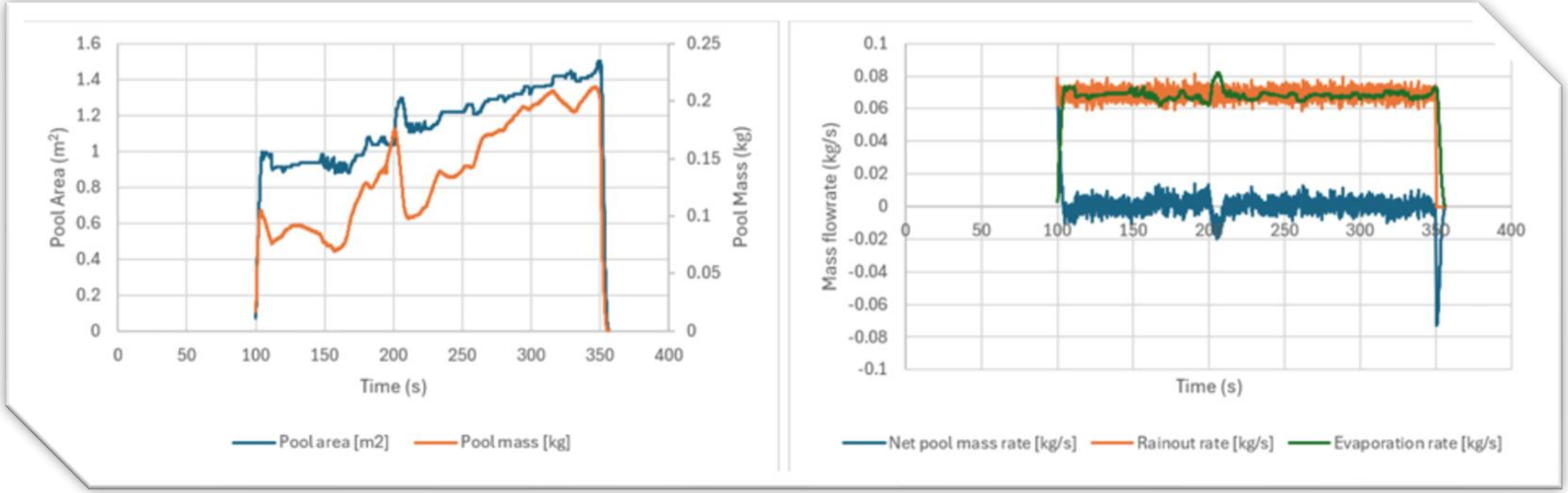
[3] D. Rescigno *et al* “Modeling of Accidental Liquid Hydrogen Spills and Rainout,” ESREL SRA-E 2025, Ed., Research Publishing, Singapore, 2025, pp. 1957–1964. doi: 10.3850/978-981-94-3281-3.

Results: LH_2 Pool Spreading and Vaporization

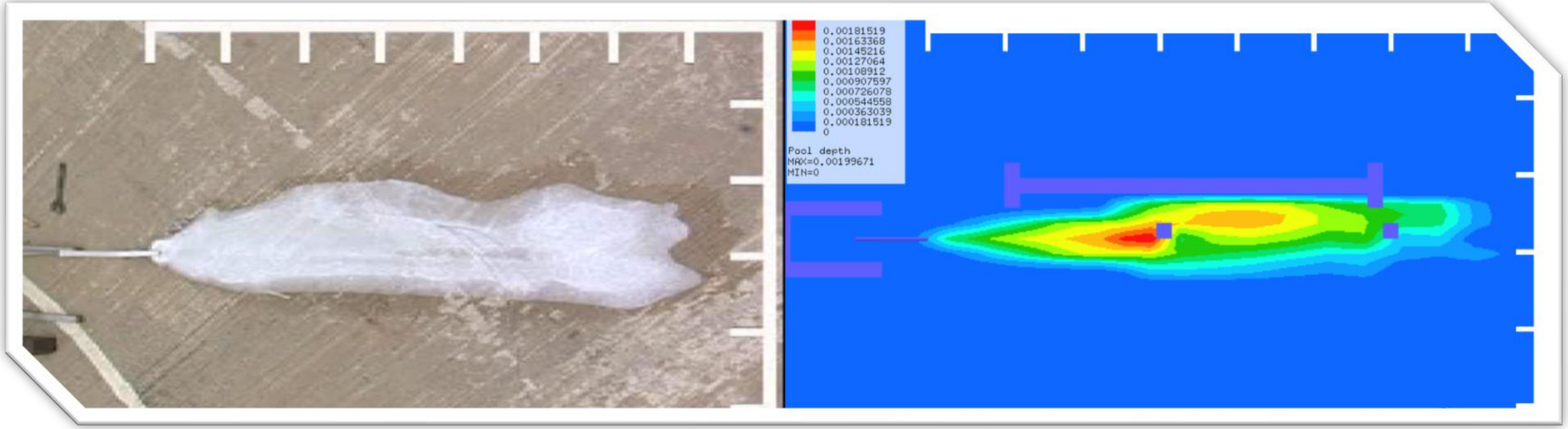
The **CFD simulation results** exhibit **good agreement** with the HSE **experimental data**:

- A **pool** with an approximate **length of 3.5 meters and a width of 0.5** meters was ultimately formed in the **simulation**.
  - ➢ In contrast, in the **experiment**, a **pool** with an approximate **length of 4 m and a width of 1 m** was observed

- **Heat transfer** from the **ground** is the **dominant contributor**, accounting for approximately **77% of the total heat input**



Pool area and pool mass over time on the left, and rainout rate, evaporation rate, and pool mass rate on the right



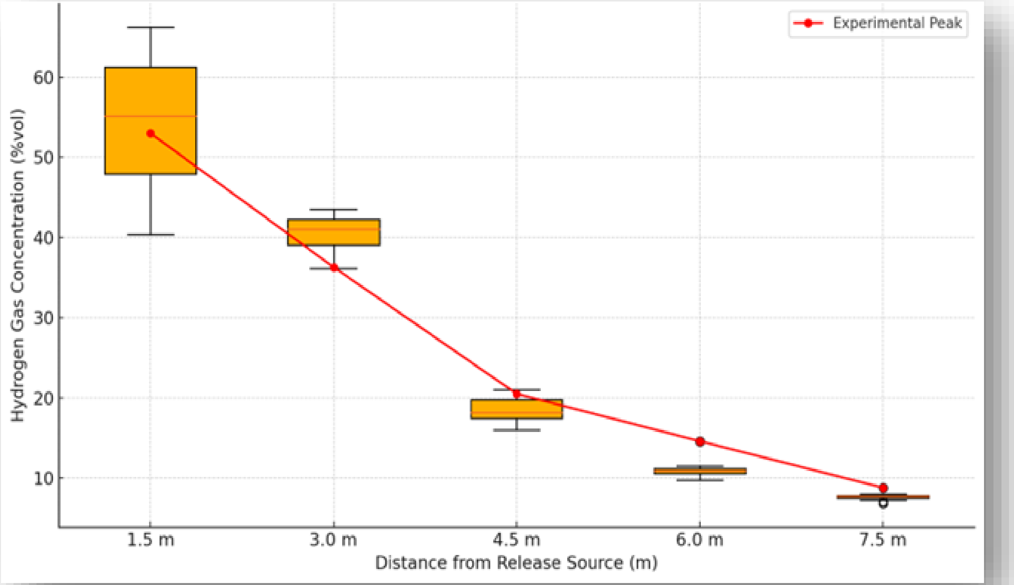
Comparison of pool shape between experiment from HSE [2] (on the left), and simulation (on the right)

Results: LH_2 Dispersion for Test 5

Comparison of gas dispersion between the experiment (on the left, [2]) and simulation (on the right)

The **iso-contour at 4.6°C**, corresponding to the dew point at a **relative humidity of 68%**, is illustrated in the **simulation**

Box plot of simulated and experimental hydrogen concentration at the monitoring points



The **general trend** of decreasing concentration with increasing distance **is well captured. However,** the **simulation results do not replicate each experimental peak in time**

Model Limitations

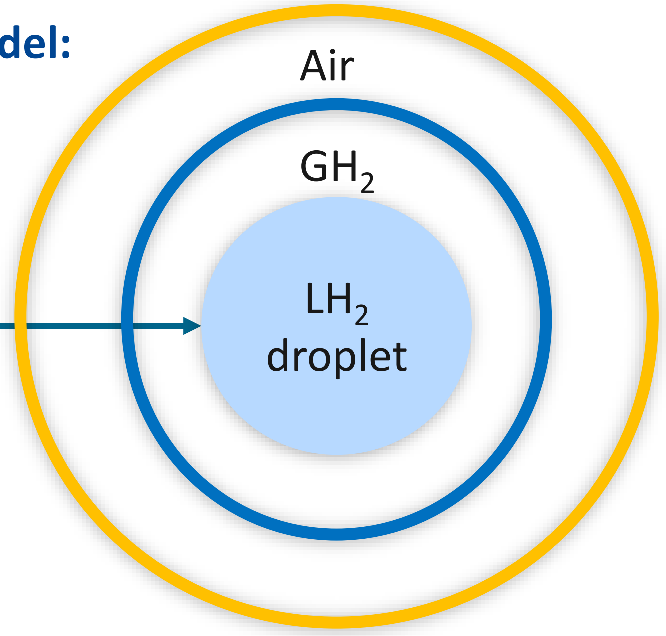
CFD software:

The CFD simulation predicted a smaller LH_2 pool than the experiment. Possible causes:

- KFX does not consider:
  1. **Film, transition, and nucleate boiling regimes**
  2. **Oxygen and nitrogen condensation** effect
  3. **Water condensation**
- Some **sensors** and **experimental supports** (e.g., mounting rod) **influenced the spreading of the pool** and the measured **concentrations**
- **Roughness** and the presence of **solidified layers** may have **altered** the spreading of the **pool**

Measurement discrepancies: differences between tabulated sensor positions and actual positions → this affected data validation

Intregral model:



Temperature of the droplet:

$$T_d = T_a - \frac{L_{v,d} \cdot k_B \cdot \rho_{Lf} \cdot \left(1 + 0.28 \cdot Re_d^{\frac{1}{2}} \cdot S_c^{\frac{1}{3}}\right)}{4 \cdot \lambda \cdot \left(1 + 0.28 \cdot Re_d^{\frac{1}{2}} \cdot P_r^{\frac{1}{3}}\right)}$$

T_a = air temperature

$$k_B = \frac{4 \cdot \mu_i \cdot D \cdot P_a}{\rho_{Lf} \cdot R \cdot T_a} \cdot ln\left(1 + \frac{P_s(T_d)}{P_a}\right)$$

Takeaways and Conclusions

- Multi-stage modeling has proven to be a **valid approach** for simulating LH_2 releases, as it largely reproduces the experimental results. However, further improvements are still required:
  - Evaporation models**: the integral model yields results similar to KFX for droplet evaporation**; however, it should be refined by using the jet temperature instead of the air temperature
  - Further studies must consider **film, transition, and nucleate boiling regimes** and **oxygen and nitrogen condensation effects** within both the integral model and CFD
- The simulated **LH_2 pool** is **slightly smaller** than in the **experiment**, but the **temporal evolution** is **well reproduced**
- **GH_2 dispersion** results remain **uncertain**, as simulations do not adequately capture the persistence of high concentrations far from the release point
- **Future experiments** must be performed using **lower pressure** at the nozzle for **horizontal releases** and **higher pressure** at the nozzle for **vertical releases**

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Thank you for your attention

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