MultHyFuel

# WP3.5 Identification of safety critical scenarios of Hydrogen Refuelling Stations in a multifuel context

*Elena Vyazmina, D. Houssin, J. Stewart, M. Ivings, C. Dixon, G. Lecocq*

September 2023

Clean Hydrogen Partnership

ICHS International Conference on Hydrogen Safety

Québec

*September 19-21, Quebec City, Canada*

*This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking under Grant Agreement No 101006794. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation programme, Hydrogen Europe and Hydrogen Europe research.*

The contents of this presentation, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy

Safety and Permitting for Hydrogen at Multifuel Retail

# MultHyFuel

"(…) lack of guidelines and instructions for local authorities can cause **delays**, **extra costs** and **divergent interpretations** from case-to-case, further complicating the obligations of HRS operators."
2018, https://www.hylaw.eu/

Definition of **commonly applicable, effective, and evidence-based guidelines** to facilitate the construction of HRS in multi-fuel refuelling stations through

- Identification of relevant gaps in the current legal and administrative framework;
- Acquisition of experimental data from engineering research;
- Active engagement with a community of stakeholders in the overall process.

Hydrogen Europe | Air Liquide creative oxygen | BESPOKE RESEARCH AND CONSULTANCY FROM HSE | INERIS maîtriser le risque pour un développement durable | ENGIE Lab CRIGEN | ITM POWER Energy Storage | Clean Fuel | kiwa | snam | Shell Hydrogen | ZSW

Clean Hydrogen Partnership

*Main objective : To develop best practice guidelines that can be used as a common approach to risk assessment, addressing the safe design for hydrogen refueling stations in a MultiFuel context:*

# MultHyFuel Project

MultHyFuel

**WP6 – Project management**

**WP1 - Detailed investigation of current status**
- T1.1 Definition of scope for regulatory analysis (Cross-country research framework)
- T1.2 Research into permitting requirements and public guidance on required risk assessments
- T1.3 Comparative assessment and gap analysis

**WP2 - Practical research to address gaps in current understanding**
- T2.1 Leakage characterisation of H2 dispensers
  - Task 2.1.1 Leakage characteristics
  - Task 2.1.2 Dispersion characteristics
  - Task 2.1.3 Ignition probabilities
  - Task 2.1.4 Efficiency of safety barrier
- T2.2 Fire and explosion hazards
  - Task 2.2.1: Defining a zoning threshold
  - Task 2.2.2 Domino effect arising from faults on hydrogen dispensers
  - Task 2.2.3 Vulnerability of hydrogen dispensers to incidents involving other fuel dispensers

**WP3 - Generate best practice guidance**
- T3.1 State of the art of technology
- T3.2 State of the art on risk assessment methodologies
- T3.3 Preliminary risk analysis
- T3.4 Detailed risk assessment
- T3.5 Identification of critical scenarios
- T3.6 Risk assessment review of critical scenarios & hazardous areas
- T3.7 Best practice guidelines redaction

**WP4 – Engagement**
- T4.1 Establishment of the Network
- T4.2 Inception phase
- T4.3 Workshop on state of the art and case study models
- T4.4 Workshop on refined case study models and WP2 methodology
- T4.5 Workshop on results of WP2 and WP3
- T4.6 Workshop on development of best practice guidance
- T4.7 Meeting on adoption of best practice guidance (WP3)

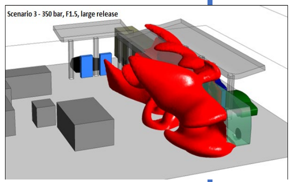
**WP5 - Dissemination, Communication and exploitation**

Paper ID219 → Task 2.1.1 Leakage characteristics

This paper → Task 2.1.2 Dispersion characteristics

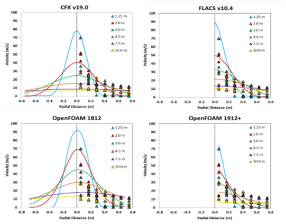
Paper ID263 → T3.4 Detailed risk assessment

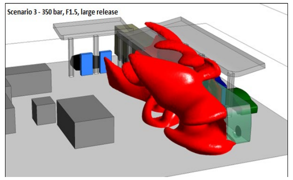
Paper ID128 → T3.6 Risk assessment review of critical scenarios & hazardous areas



# 2. Scope of the work

MultHyFuel



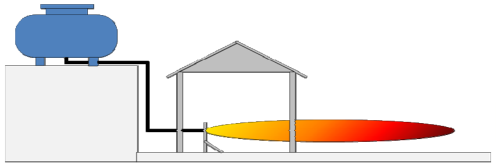

Two stages as follows:

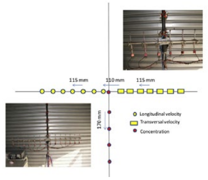
- Model Validation – to evaluate CFD models performance by comparison with experiments.
- Realistic Release Modelling – to perform demonstration simulations for critical scenarios.

**Model Validation Cases**

- *Unobstructed Non-Confined Jet* (outside dispenser):

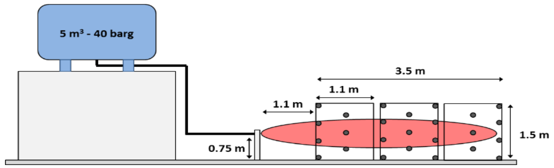
  m=0.26kg/s, D=12m, P=35barg, $T_{gas}$=35°C, $T_{amb}$=10°C, h=1.5m above the ground





- *Obstructed Not-Confined Jet* (outside dispenser)

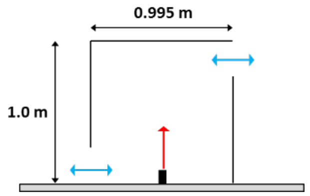
  m=0.26kg/s, D=12m, P=38barg, $T_{gas}$=9°C, $T_{amb}$=15°C, h=0.75m above the ground

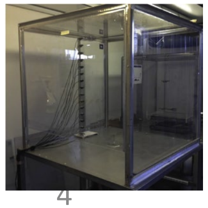



- *Confined Release* (inside dispenser)

  1m³, flow rates 10.4 & 218.3 NL/min, D=27m, $T_{gas}$=$T_{amb}$=12°C, h=80mm above the base

  2 openings of w=960 mm h=180 mm



Clean Hydrogen Partnership

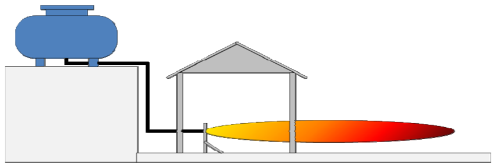
# 3. Models and Approaches

| | FLACS v10.4/10.6 | CFX v19.0 | OpenFOAM v1912+ | OpenFOAM v1812 |
|---|---|---|---|---|
| **Unobstructed Free Jet** | | | | |
| Mesh Type | Structured Cartesian | Unstructured tetrahedral | Structured Cartesian | Hexahedral with mesh adaptation |
| Grid at Inlet BC | 1 cell | 108 nodes | 10 cells | 44 faces |
| Mesh Node Count | 4,179,175 | 1,956,404 | 9,100,000 | 1,401,218 |
| Domain Dimensions | 65 m x 30 m x 17 m | 22 m x 6 m x 5 m | 20 m x 8 m x 5 m | 17 m x 10 m x 8 m |
| **Obstructed Free Jet** | | | | |
| Mesh Type | Structured Cartesian | Unstructured tetrahedral | Structured Cartesian | Hex dominant with mesh adaptation |
| Grid at Inlet BC | 1 cell | 115 nodes | 6 cells | 52 faces |
| Mesh Node Count | 2,664,750 | 2,589,006 | 2,100,000 | 2,337,376 |
| Domain Dimensions | 17 m x 14 m x 8.1 m | 22 m x 8 m x 5 m | 8.5 m x 4 m x 4 m | 17 m x 10 m x 5 m |
| **Confined Releases** | | | | |
| Mesh Type | Structured Cartesian | Unstructured tetrahedral | Structured Cartesian | Hexahedral with mesh adaptation |
| Grid at Inlet BC | 1 cell | 120 nodes | 6 cells | 24 faces |
| Mesh Node Count | 891,075 | 1,014,353 | 1,000,000 | 2,765,550 |
| Domain Dimensions | 1.96 m x 1.38 m x 1.75 m | 4 m x 4 m x 2.5 m | 4 m x 4 m x 2 m | 8 m x 9 m x 6 m |

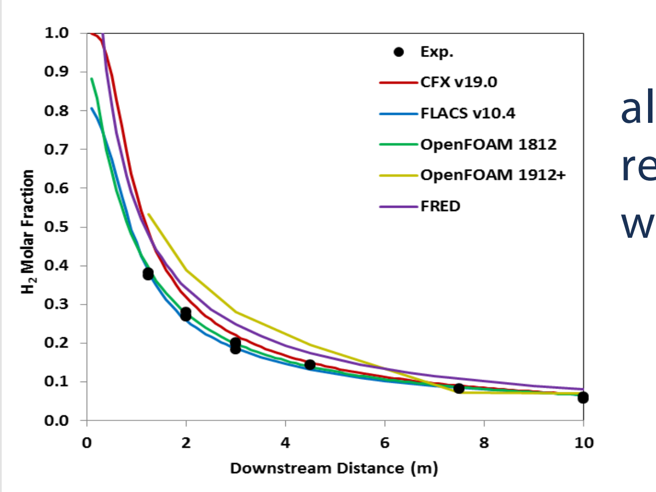
| | Unobstructed | Obstructed | Unobstructed | Obstructed |
|---|---|---|---|---|
| **CFD Model** | **FLACS v10.4** | | **OpenFOAM 1812** | |
| Source Model | FLACS Jet Program | | FRED | |
| Diameter (mm) | 74.0 | 74.0 | 68.0 | 72.0 |
| Velocity (m/s) | 704.6 | 704.6 | 775.0 | 768.0 |
| Temperature (K) | 280.7 | 280.7 | 255.6 | 245.9 |
| $H_2$ Mass Fraction | 1.0 | 1.0 | 0.894 | 0.895 |
| **CFD Model** | **CFX 19.0** | | **OpenFOAM 1912+** | |
| Source Model | Ewan & Moodie [15] | | EXORIS Model | |
| Diameter (mm) | 51.2 | 54.0 | 46.4 | 48.9 |
| Velocity (m/s) | 1199.5 | 1164.8 | 1170.0 | 1170 |
| Temperature (K) | 247.4 | 233.3 | 248.0 | 225.0 |
| $H_2$ Mass Fraction | 1.0 | 1.0 | 1.0 | 1.0 |

For more details about models, see the paper

# 4. Model Validation Results: unconfined

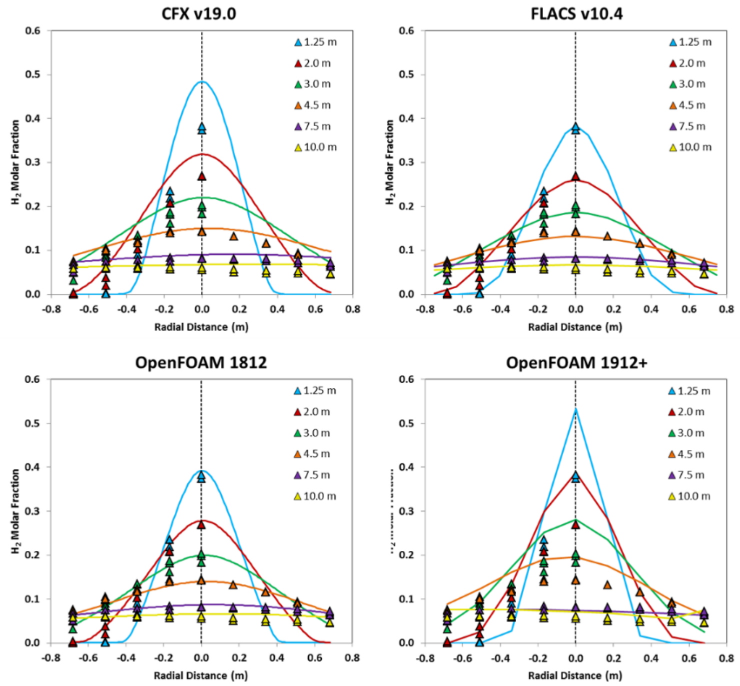


Centerline $H_2$ molar fraction




all the models are in reasonable agreement with the exp

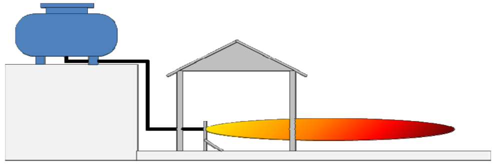
Radial distribution of the $H_2$ molar fraction



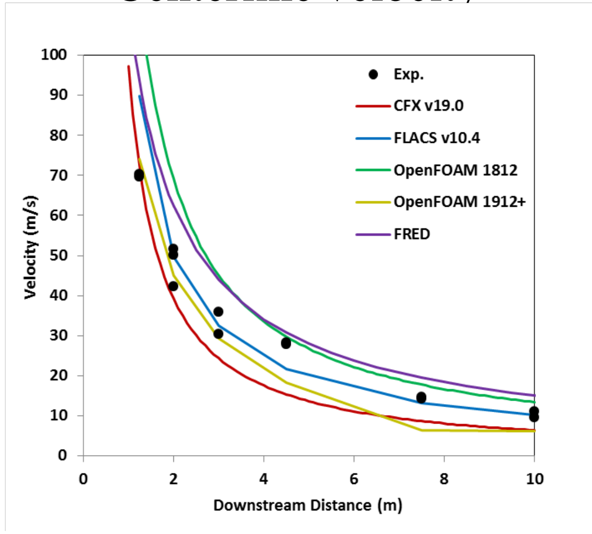

- **FRED**: over-prediction ➔ conservative approach
- **FLACS**: good agreement
- **CFX**: reasonable agreement for the width and concentrations starting from 3m
- **OpenFOAM 1812**: excellent agreement along the centerline, slight under-prediction close to release
- **OpenFOAM 1912+:** significant overprediction at the centerline, good agreement with the jet widths

NB: OpenFOAM results are different due to modeling approach, not due to the difference in version

# 4. Model Validation Results: unconfined

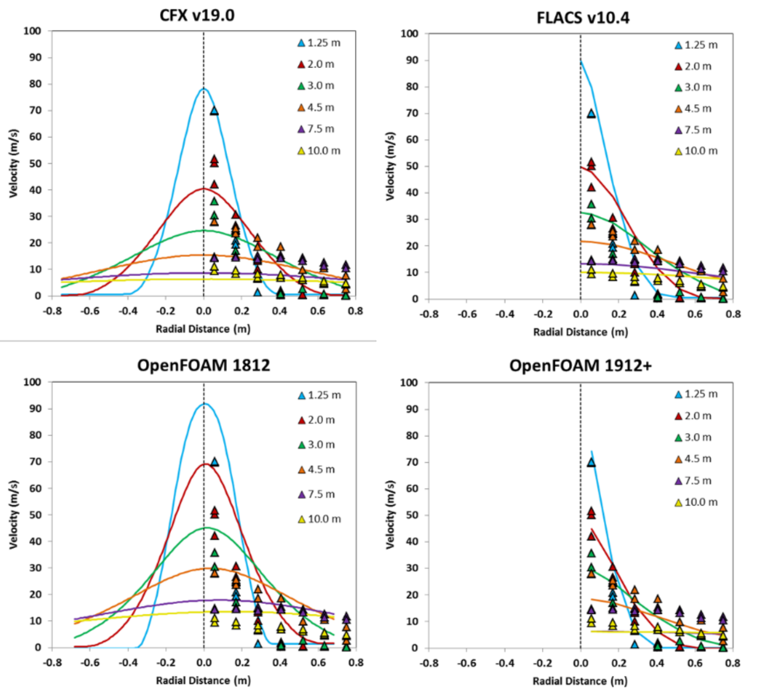


Centerline velocity



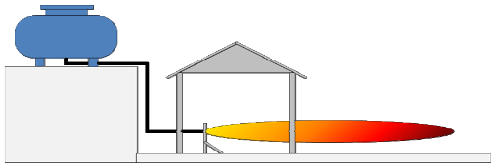

All the models are in reasonable agreement with the experiment starting from 4m

Radial distribution of the velocity

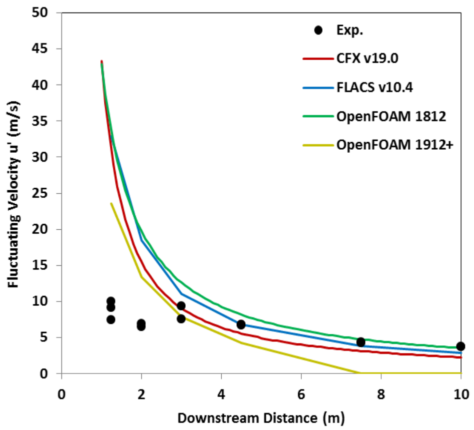



- **FRED** close to OpenFOAM 1812 (overestimation of the velocity)
- **OpenFOAM 1812**: good approximations of the jet width except at 4.5m, but over-predicts the centerline velocity
- **FLACS, CFX & OpenFOAM 1912+** : under-predict the centerline velocity and the jet width at 4.5 m
- **FLACS**: in good agreement in general
- **CFX**: reasonable approximation of the jet widths
- **OpenFOAM 1912+**: good agreement with the jet widths and the centerline velocity measurements

# 4. Model Validation Results: unconfined

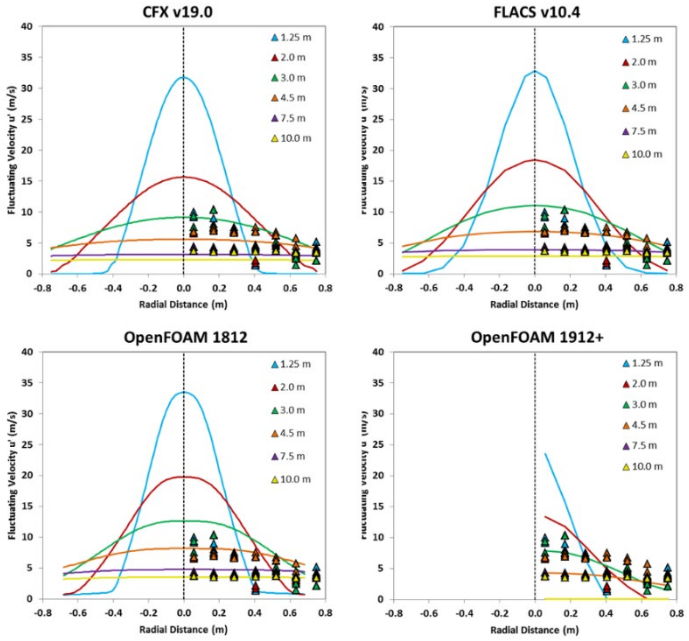


Centerline fluctuation velocity



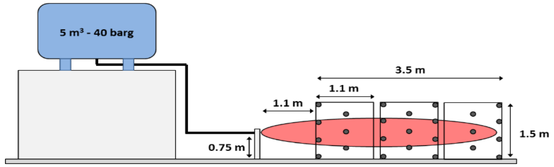

All the models are in reasonable agreement with the experiment starting from 4m

Radial distribution of the fluctuating velocity



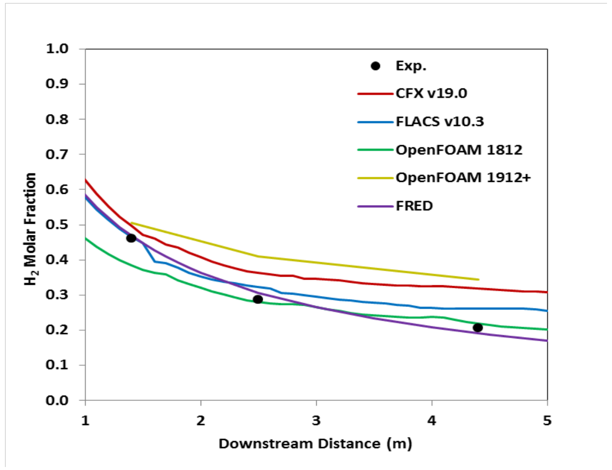

- **CFX, FLACS** and **OpenFOAM 1812**
- In the nearfield over-predicted u’ (saturation of the velocity sensor)
- Good agreement with the measured data at distances of 4.5 m and further
- **OpenFOAM 1912+** gives zero turbulent fluctuating velocity at 7.5 m and further

# 4. Model Validation Results: unconfined

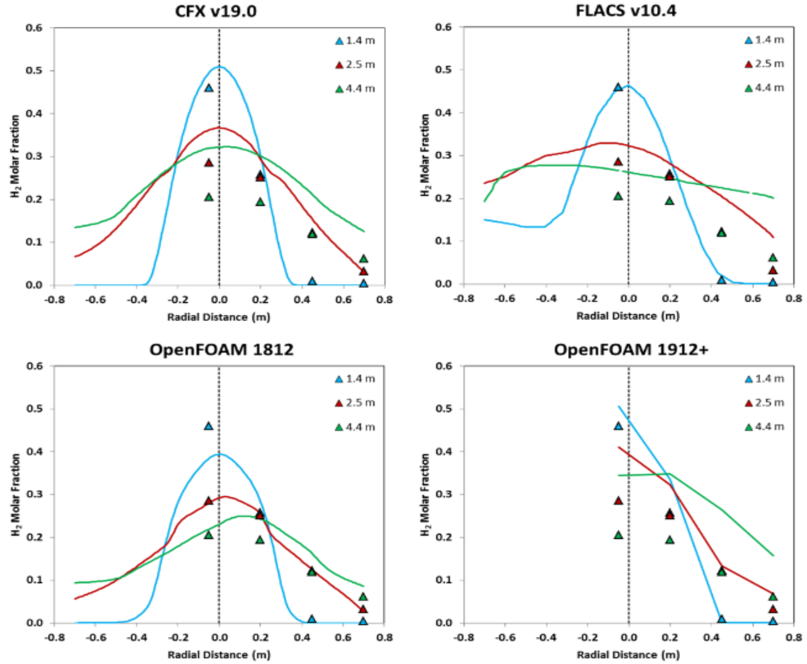



MultHyFuel

Centerline $H_2$ molar fraction



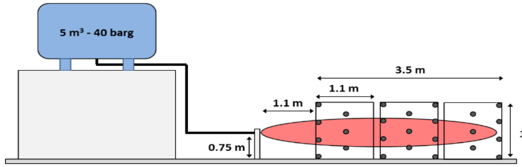

Radial distribution of the $H_2$ molar fraction



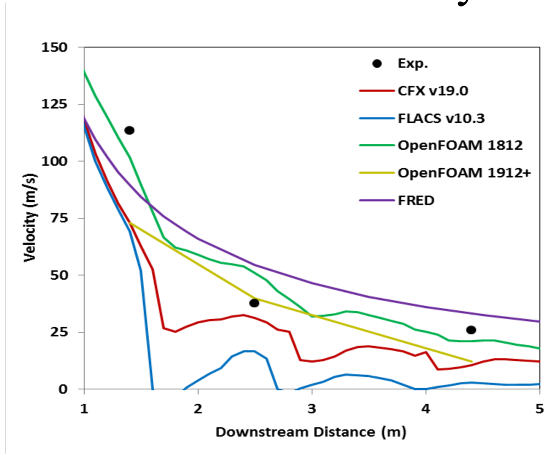

- **CFX** over-predict the concentrations
- **FLACS** over-predicts concentrations and jet widths further downstream
- **OpenFOAM 1812** under-predicts the concentration at the first location and give excellent agreement further downstream, jet width is well caputed
- **OpenFOAM 1912+** represents well jet widths but over-predicts the specific concentration
- **FRED** results give the closest agreement with the measured data.
- **CFX, FLACS and OpenFOAM 1812** predicts asymmetry of the jet in the radial profiles.

NB: geometry representation by PDR is not the most appropriate for round bars with a size similar to the mesh

# 4. Model Validation Results: unconfined

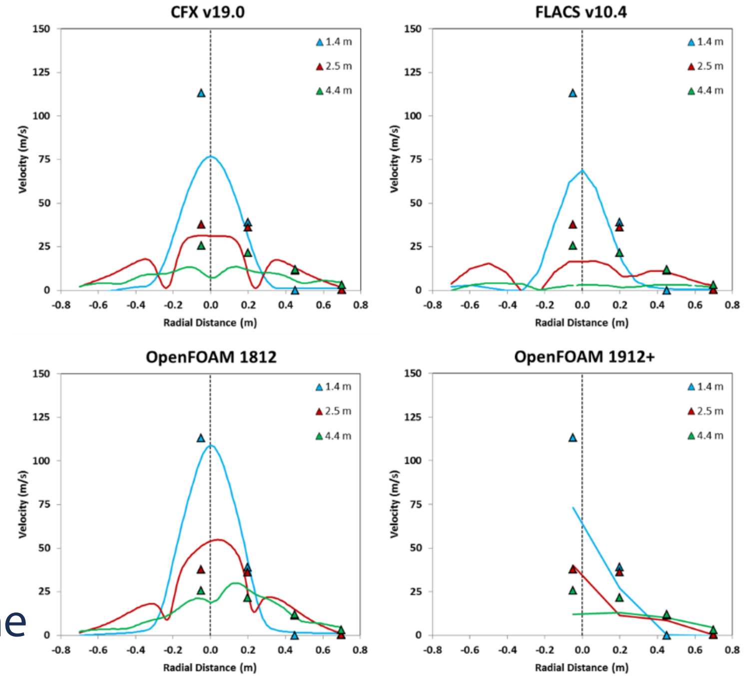



Centerline velocity




All the models capture the jet width relatively well, as shown by predictions of radial velocity profiles.

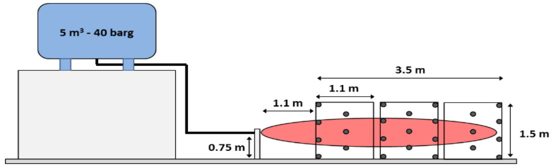
Radial distribution of the velocity



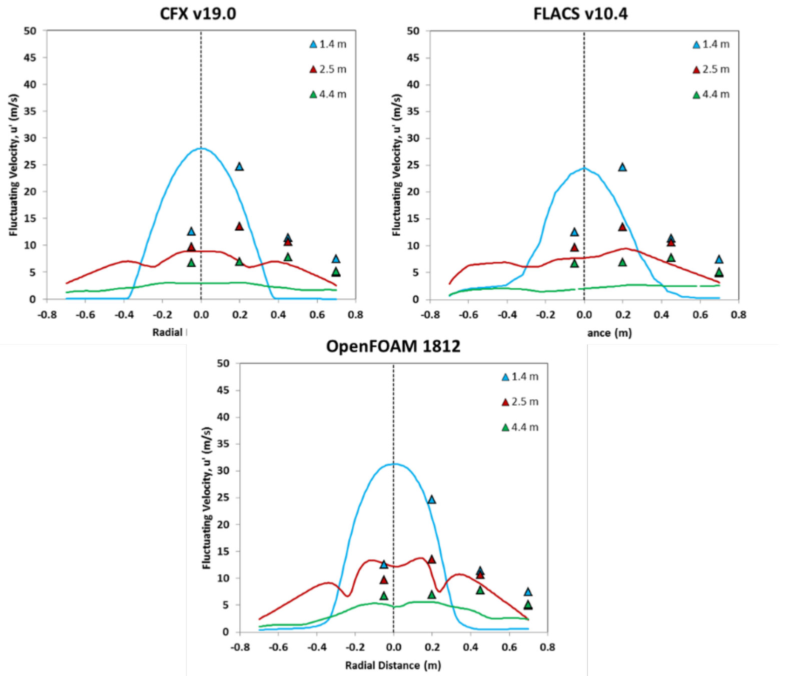

- **OpenFOAM 1812** & **1912+** and **FRED** are in better agreement at the centerline
- **CFX** & **FLACS** significantly underestimate the centerline velocity
- **CFX, FLACS, OpenFOAM 1812 :** the centerline decay showing drops in velocity due to the interactions between the jet and the obstacle array. Similarly, in the radial velocity profiles at 2.5 m and 4.4 m from the release point, all three models show drops in velocity either side of the centerline, because of the obstacles.
- **FRED** predictions bisect the measured data points, initially under-predicting at 1.4 m and over-predicts the centerline velocity for the other two measurement locations.

NB: geometry representation by PDR is not the most appropriate for round bars with a size similar to the mesh

# 4. Model Validation Results: unconfined



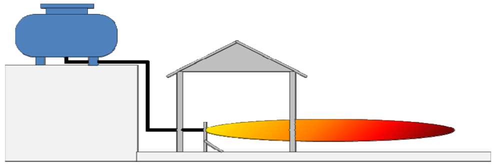

Radial distribution of the fluctuating velocity

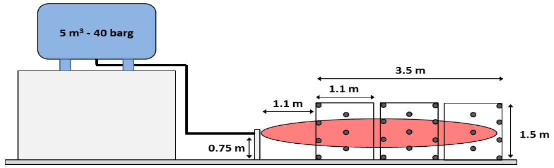



- **CFX, FLACS & OpenFOAM 1812** show asymmetry across the radial profiles
- **OpenFOAM 1812** is the closest agreement with the experiment
- **FLACS** significantly underestimates the fluctuation velocity

NB: geometry representation by PDR is not the most appropriate for round bars with a size similar to the mesh

# 5. Source term influence

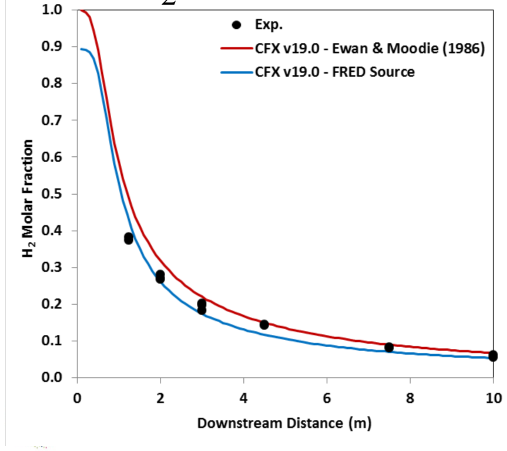




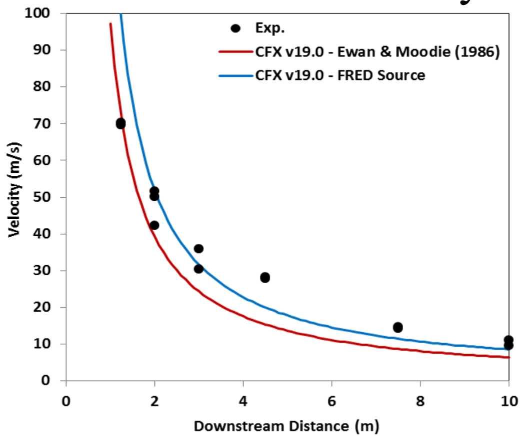

- The choice of source term has a reasonable influence on the results
- CFX in closer agreement with exp. using the source term generated with FRED than with the Ewan and Moodie one

- CFX with the source conditions taken from FRED gives closer agreement with the measured data, similarly to the findings for the unobstructed jet case

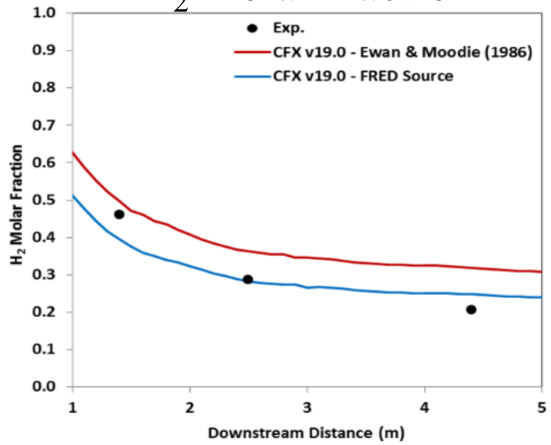
$H_2$ molar fraction



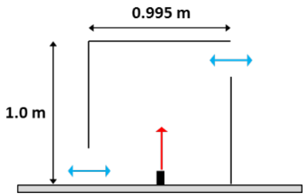

Centerline velocity

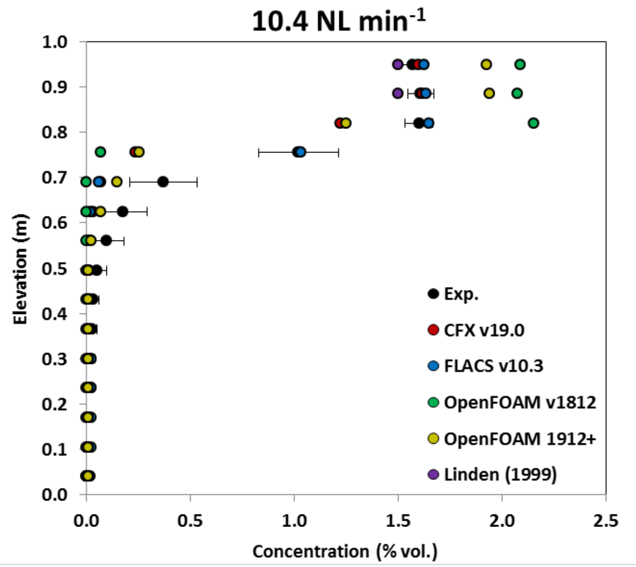


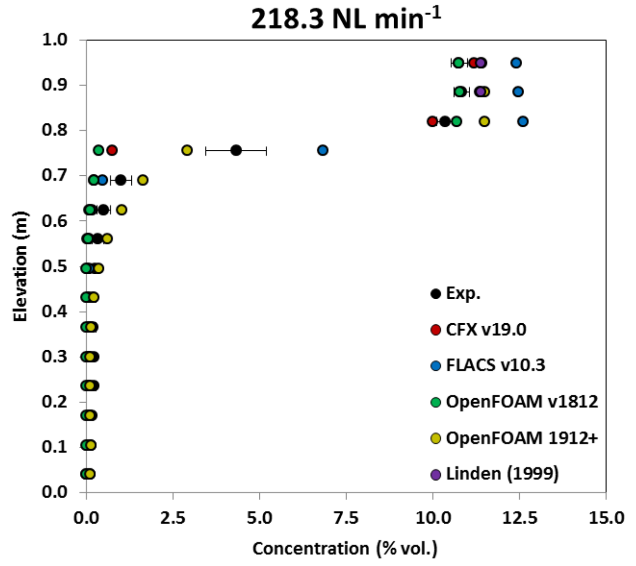

$H_2$ molar fraction



# 6. Model Validation Results: confined




- For both releases & all models, the predicted concentrations in the transition layer (0.6-0.8 m) shows less good agreement with the measured data than in the other parts of the confinement
- **Linden** is in good agreement with the experiment
- For the 218.3 NL min-1 release,
  - ➔ all models give good estimation of the concentration at the upper layer
  - ➔ closer agreement between the model predictions and the measured concentrations
- For the 10.4 NL min-1 release,
  - ➔ **CFX**, **FLACS** & **Linden** give a good estimation of the concentration at the upper layer
  - ➔ **OpenFOAM**s overpredicts the upper layer concentration
  - ➔ **OpenFOAM 1912+** & **CFX** underpredict the thickness of the upper layer (concentration underprediction at 0.8m)

# 7. Conclusion & Recommendation

MultHyFuel

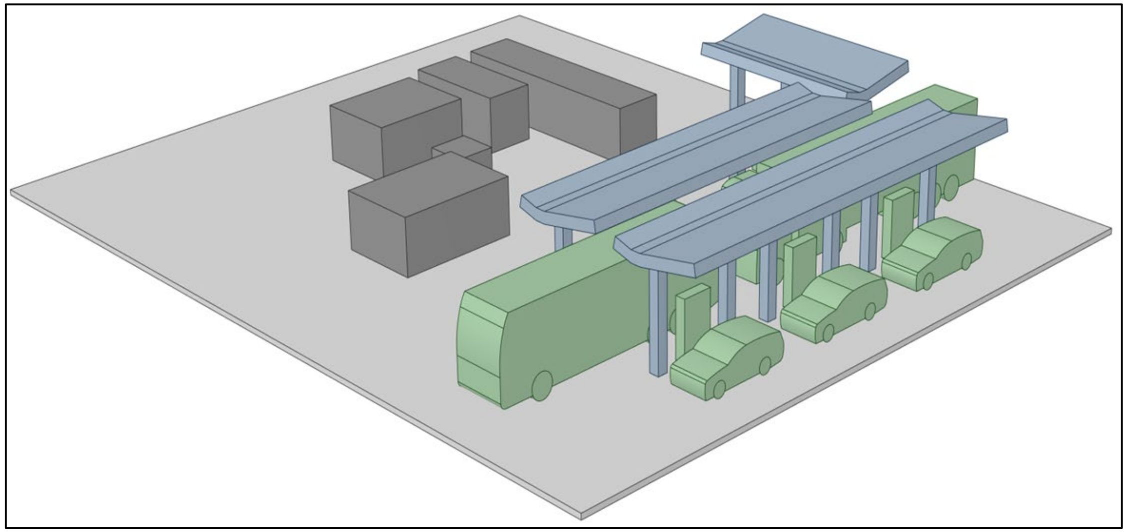
- **Conclusions:**
  - CFD approaches selected by the partners can **reasonably reproduce the measured data** across the selected range of the considered scenarios (however validation results show some scatter in predictions, with both overprediction and underprediction) ➔ the models produce acceptable solutions for the realistic release modelling
  - The specification of the **source term is important** and influences the dispersion results

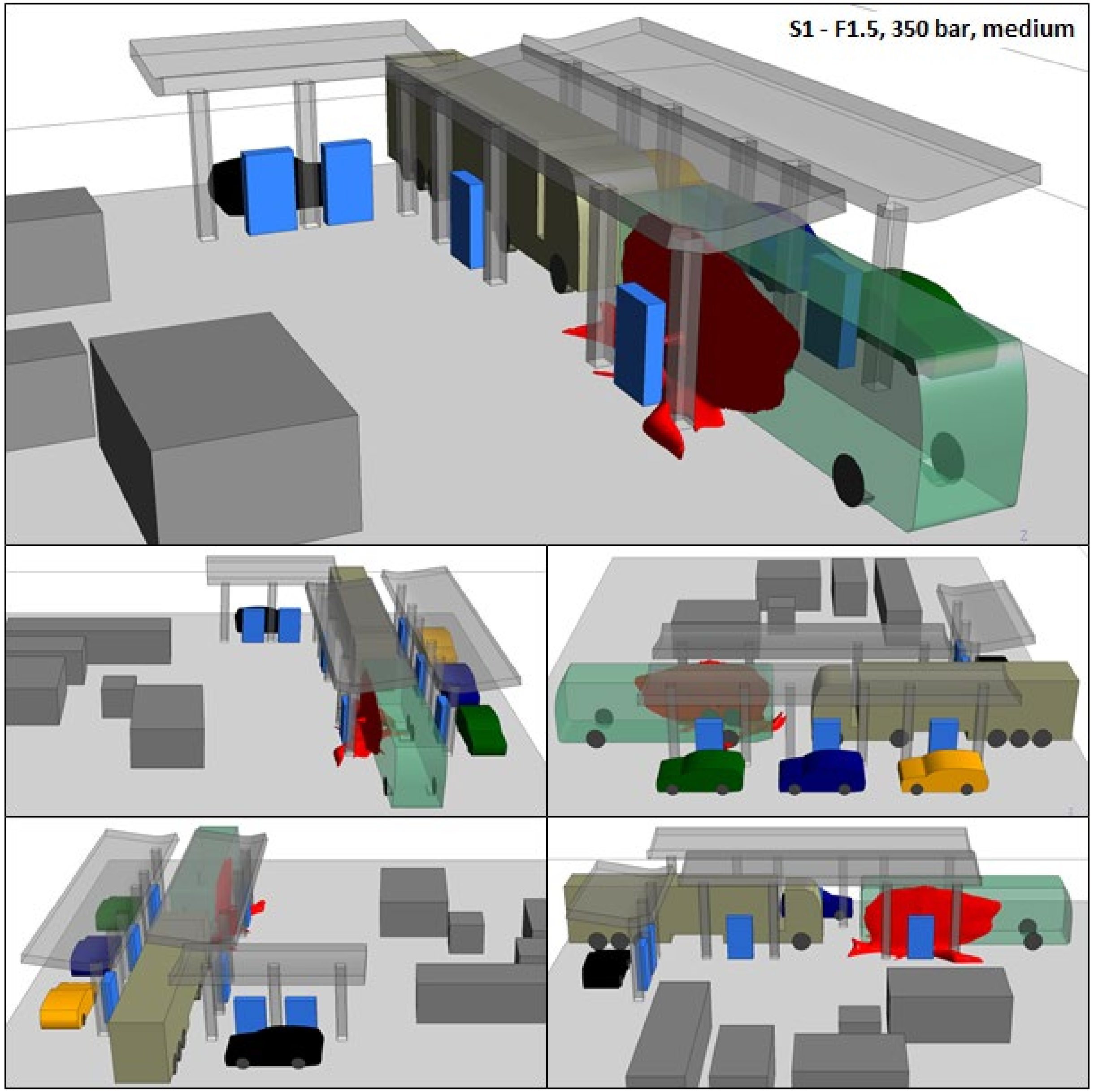
- **Recommendations:**
  - Before performing a dispersion computation for realistic cases, the **CFD approach shall be validated vs simple cases** to find out any drawback of models and identify the appropriate approach. <u>It is essential</u> to avoid to go directly to realistic cases without <u>validation</u>
  - ***A suitable jet model*** is used for jet simulations to estimate the conditions within the expanded jet where the local Mach number is 1, or just below. These conditions can then be used to specify inlet conditions for CFD calculations.

Clean Hydrogen Partnership

# 8. Realistic Release Modelling

- <u>Only Validated</u> models can be used for realistic prediction






- ➔ this is another story

# Thank you for your attention!

info@multhyfuel.eu

MultHyFuel

*This project has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking under Grant Agreement No 101006794. This Joint Undertaking receives support from the European Union's Horizon 2020 Research and Innovation programme, Hydrogen Europe and Hydrogen Europe research.*