DETAILED ASSESSMENT OF DISPERSION FOR HIGH-PRESSURE H2 IN MULTI-FUEL ENVIRONMENT

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ABSTRACT

The MultHyFuel project notably aims to produce the data missing for usable risk analysis and mitigation activity for Hydrogen Refuelling Stations (HRS) in a multi-fuel context.
In this framework, realistic releases of hydrogen that could occur in representative multi-fuel forecourts were studied. These releases can occur inside or outside fuel dispensers and they can interact with a complex environment notably made of parked cars and trucks. This paper is focused on the most critical scenarios that were addressed by a sub-group through the use of Computational Fluid Dynamics (CFD) modelling. Once the corresponding source terms for hydrogen releases were known, two stages are followed:

- Model Validation – to evaluate the CFD models selected by the task partners and to evaluate their performance through comparison to experimental data.
- Realistic Release Modelling – to perform demonstration simulations of a range of critical scenarios.

The CFD models selected for the Model Validation have been tested against measured data for a set of experiments involving hydrogen releases. Each experiment accounts for physical features that are encountered in the realistic cases. The selected experiments include an under-expanded hydrogen jet discharging into the open atmosphere with no obstacles or through an array of obstacles. Additionally, a very different set-up was studied with buoyancy-driven releases inside a naturally ventilated enclosure. The results of the Model Validation exercise show that the models produce acceptable solutions when compared to measured data and give confidence in the ability of the models, and the modellers, to capture the behaviour of the realistic releases adequately.
The Realistic Release Modelling phase will provide estimation of the flammable gas cloud volume for a set of critical scenarios and will be described at the second stage.

Keywords: *Critical scenarios, dispersion, CFD models, validation*

INTRODUCTION

The MultHyFuel project [1] funded by the Clean Hydrogen Partnership is dedicated to effective and safe deployment of Hydrogen Refuelling Stations (HRS) in a multi-fuel context.
The preliminary risk assessment of HRS in a multi-fuel context for three typical configurations [2] demonstrated the need of the Computational Fluid Dynamics (CFD) modelling for the most critical scenarios identified. The current modeling work gives a prediction of flammable cloud volumes and masses.
The work has been conducted in 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.

The current work concerns the Model Validation exercise, whereas the Realistic Release Modelling will be performed in a second step.

CFD MODEL VALIDATION

Model Validation Cases

Unobstructed Non-Confined Jet

Daubech et al. [3] performed a series of horizontally oriented unobstructed free jet releases of H_2 through a 12 mm diameter nozzle located 1.5 m above the ground. Temperature (25.0$\pm$1.0 °C) and pressure (34.0$\pm$0.1 barg) were measured just upstream of the nozzle exit. Repeatability tests were performed. The ambient temperature was 10°C. The fields of H_2 concentration, velocity and turbulence intensity were measured at discrete locations in the area where the jet could develop itself. For more information concerning the experimental description, see [3-6].

Whilst the release pressure for the free jet tests modelled here is substantially lower than expected for an HRS dispenser, the resulting mass flow rate of H_2 is quite similar to the highest dispensing flow rate envisioned of 300 g/s for a heavy-duty dispenser.

Obstructed Not Confined Jet

The unobstructed jet tests described by [3-6] were performed within the ExJet Joint Industry Project. Within ExJet, a series of obstructed jet releases at similar conditions (the temperature 8.0$\pm$1.0 °C and pressure 38.0$\pm$0.1barg, ambient temperature15°C) were also undertaken [7]. The jet was directed into an obstacle array comprising numerous 1.5m long, 0.1m diameter cylinders, spaced approximately 0.35m apart in the vertical direction, oriented perpendicularly to the jet flow (see Figure 1).

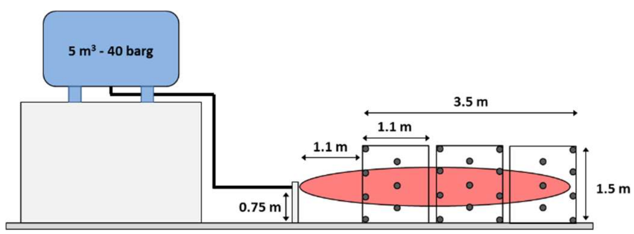

Figure 1 – Schematic of the experimental setup used for the obstructed free jet releases

On a multi-fuel forecourt, numerous obstacles could be present in the path of a flammable cloud generated by an accidental release, for example the dispenser casing, vehicles and any building structures such as the fuel station shop. Hence it is critical that the model performance is assessed for cases with obstructions (there are not many available experiments with hydrogen for such releases).

Confined Release

A series of confined H_2 releases [8] were performed inside naturally ventilated 1 m^3 enclosure (1 m high with a 0.995 m square base). H_2 was released vertically from a 27.2 mm internal diameter pipe 80 mm above the enclosure base. The flow rates of 10.4 and 218.3 NL min^{-1} were imposed, the temperature was 12°C. The enclosure included two ventilation openings, one at the top and the other at the bottom of two opposing walls, each 960 mm wide and 180 mm high (see Figure 2). Measurements of H_2 concentration were carried out along the vertical line (see [8-9] for more details).

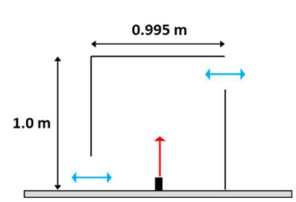

Figure 2 – Schematic of the confined release test configuration

Validation of the CFD models for confined releases is necessary to check they could capture the physics associated with realistic releases inside the dispenser casing.

CFD Models and Approaches

The predictions of AEROPLUME [11], which is a part of the FRED [10] package, were compared to the CFD and experimental results.

Each partner has selected different CFD model(s), or version(s): CFX v19.0 [12] (HSE), OpenFOAM v1912+ [13] (INERIS), OpenFOAM v1812 [13] (Shell), FLACS v10.4 & v10.6 [14] (Air Liquide).

Modelling high-pressure, under-expanded jet releases directly from the orifice presents a significant challenge numerically. Hence, so-called *pseudo-source* or *notional nozzle* approaches, which can approximate the jet conditions downstream of the shock structure are usually used. This substantially reduces the computational mesh size requirement, and consequently the simulation run time. The source terms used by the modellers for the hydrogen release are described in Table 1.

	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

Table 1 – Summary of the pseudo-source inlet conditions used in the different CFD models evaluated

Table 2 summarises the computational domain dimensions and mesh characteristics selected by each task partner. There are significant differences between the approaches used with regards to the type of mesh and the mesh resolution for modelling the inlet boundary condition (BC). Both of these choices depend on the CFD model. For example, the FLACS grid guidelines stipulate the mesh resolution required for simulating a jet release, whereas the model user has more choice on how best to resolve the inlet BC in the other CFD models used in the present study. A mesh sensitivity analysis was undertaken by all participants to ensure that the model predictions are not affected by the choice of computational grid. The grid sensitivity analysis results are not presented here.

	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

Table 2 – Summary of the computational domain dimensions and mesh characteristics used with each CFD model for the three model validation scenarios studied

More information about solvers and numerical sub-models can be found in [16].

Model Validation Results

Unobstructed Non-Confined Jet

Figure 3 shows a comparison of the measured and predicted centreline H_2 molar fraction [3].

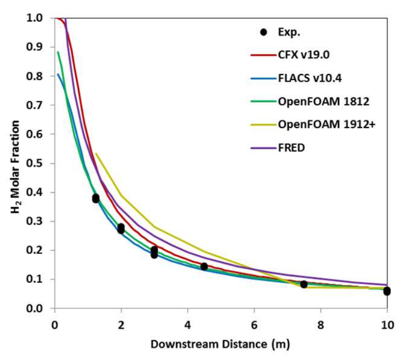

Figure 3 – Comparison of measured and predicted centreline H_2 molar fraction for the unobstructed free jet

Overall, all the models are broadly in reasonable agreement with the measurements of centreline H_2 molar fraction. However, there is less agreement between the models and the measurements for the radial profiles of H_2 molar fraction as shown in Figure 4. To summarize:

- The CFX simulation over-predicts the centerline concentration and under-predicts the jet width at the first measurement location (1.25 m and 2 m downstream from the release), but then gives better agreement with both the jet width and concentrations moving further away from the release.
- The FLACS predictions give very good agreement with the measured data at all measurement locations along the jet centerline as well as for jet widths.
- The OpenFOAM 1812 simulation also gives predictions in excellent agreement with the measured data along the jet centerline, but slightly under-predicts the jet width at the first measurement location.
- The OpenFOAM 1912+ prediction gives good agreement with the measured jet widths at most measurement locations but over-predicts the centerline concentrations significantly.

- FRED calculations over-predict the measured data and thus give a conservative estimate of the H_2 concentration along the jet centerline.

Clearly the two versions of OpenFOAM give different predictions of centreline concentration. This is likely a result of the choice of computational grid, source term and the model set up (see Table 2), rather than any substantial differences between the two versions of the CFD code.

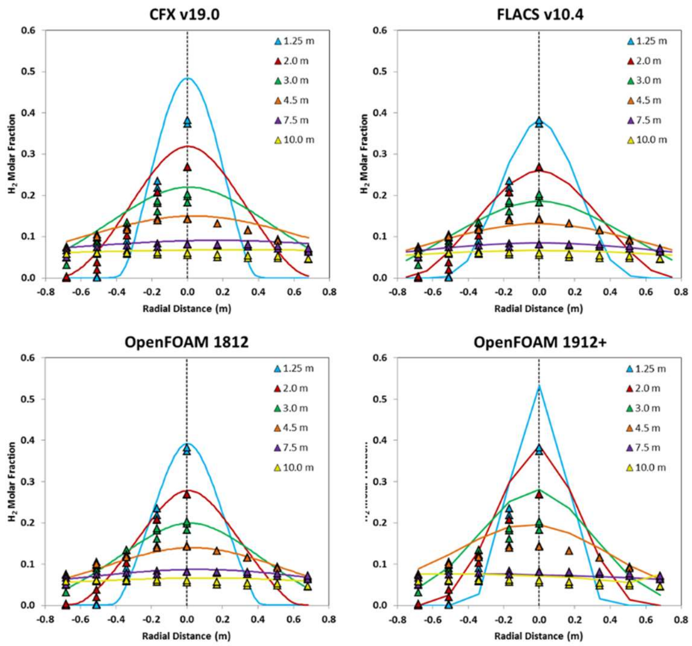

Figure 4 – Comparison of the measured (symbols) and predicted (lines) radial profiles of H_2 for the unobstructed jet scenario

Figure 5 compares the measured and predicted velocities along the centreline and Figure 6 shows a comparison of the measured and predicted velocity radial profiles. Overall, the model predictions bound the experimental data on both sides, giving both over- and under-prediction of the measured data. The velocity sensors used experimentally were saturated at distances less than 3 m from the release, and thus there is some uncertainty in the measured data at those sensors.

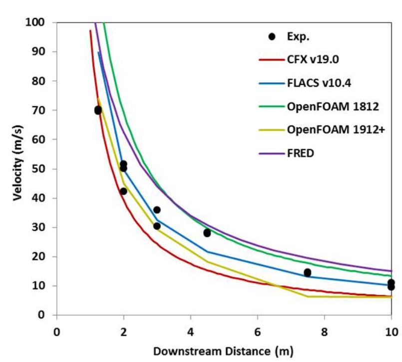

Figure 5 – Comparison of measured and predicted centreline velocity for the unobstructed free jet

Overall:

- The CFX results give reasonable approximation of the jet widths (based on velocity) and the value on the centerline for measurements to 3 m downstream of the release point (upstream of 3m the measurements are unreliable). Beyond this, the jet width is over-predicted, most notably at a distance of 4.5 m downstream of the release.

- The FLACS modelling gives generally good agreement with the measured data but under-predicts the centerline velocity and the jet width at 4.5 m measurement point from the release. The latter is common for OpenFOAM 1912+ and CFX.
- The OpenFOAM 1812 simulations over-predict the centerline velocity at all measurement locations, but give good approximations of the jet widths, except at 4.5 m downstream of the release, as for the other models.
- The OpenFOAM 1912+ predictions give good agreement with the jet widths and the centerline velocity measurements. Although, as for the other model results, the jet width at 4.5 m downstream of the release is over-predicted.
- The predictions made using the AEROPLUME jet dispersion model in FRED are very similar to those obtained with OpenFOAM 1812. This model bounds the experimental data on the upper side.

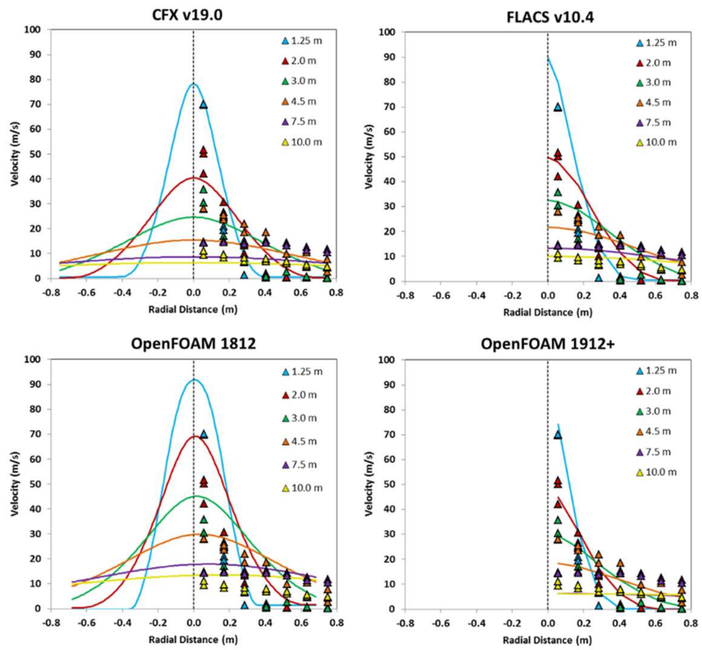

Figure 6 – Comparison of the measured (symbols) and predicted (lines) radial velocity profiles for the unobstructed jet scenario

Figure 7 and Figure 8 present comparisons between the measured and predicted fluctuating velocity component, u' (m/s) along the jet centreline and radially within the jet, respectively:

- The predictions made using CFX, FLACS and OpenFOAM 1812 are comparable and give good agreement with the measured data at distances of 4.5 m and more downstream of the release. In the nearfield, these models significantly over-predict u'. This could be due to saturation of the velocity sensors used in the experiment, thus giving uncertain results in the near field.
- The results obtained with OpenFOAM 1912+ are initially in line with the other model predictions before dropping away to give zero turbulent fluctuating velocity at downstream distances of 7.5 m and greater.

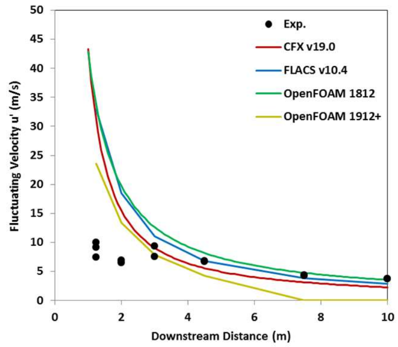

Figure 7 – Comparison of measured and predicted centreline turbulent fluctuating velocity, $\mathbf{u'}$*, for the unobstructed jet*

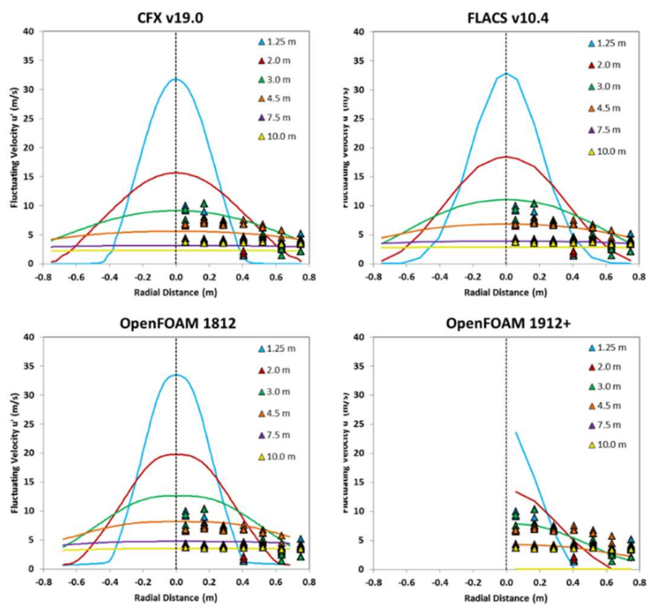

Figure 8 – Comparison of the measured (symbols) and predicted (lines) radial profiles of turbulent fluctuating velocity for the unobstructed jet scenario

Figure 9 compares the fractional turbulence intensity from the experiment and model predictions.

- Three models (FLACS, CFX, OpenFOAM 1812) are fairly similar: OpenFOAM 1812 shows a near-constant fractional turbulent intensity of around 0.27 at all measurement locations. The CFX predictions give a fractional turbulence intensity of 0.43 at the first measurement location, before this value drops to a near-constant value of 0.36. The FLACS predictions give a fractional turbulence intensity around 0.37 at the first two measurement locations downstream of the release, before the turbulence intensity decays to a near-constant value of 0.30.
- The OpenFOAM 1912+ calculations give a fractional turbulence intensity which starts at around 0.32 at 1.25 m from the release point, before the turbulence intensity decays to zero 7.5 m downstream of the release, this could be a sign of the problem in calculations.

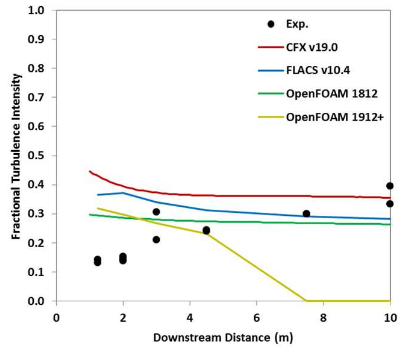

Figure 9 – Comparison of measured and predicted centreline fractional turbulence intensity for the unobstructed jet

CFX was used with source conditions estimated using both the Ewan and Moodie [15] approach and using outputs from the Shell FRED model. Figure 10 shows that the choice of source term has a reasonable influence on the results, with CFX giving predictions closer to the measured data when using the source term generated with FRED than with the Ewan and Moodie.

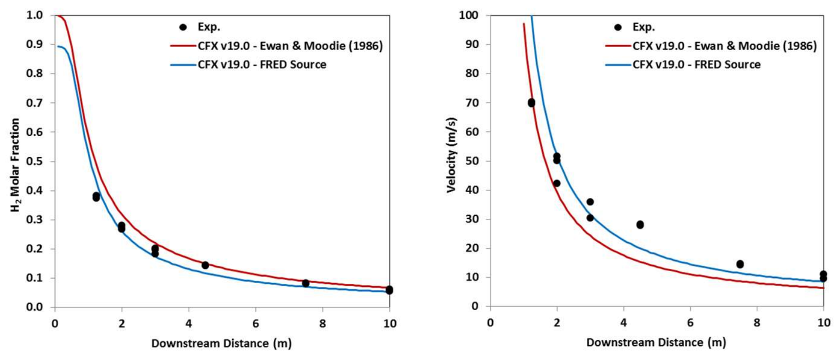

*Figure 10 – **On the left**: Comparison of the measured centreline H_2 molar fraction for the unobstructed free jet to CFX v19.0 predictions using the Ewan and Moodie [15] and Shell FRED pseudo source inlet conditions listed in Table 1. **On the right**: Comparison of the measured centreline velocity for the unobstructed free jet to CFX v19.0 predictions using the Ewan and Moodie [15] and Shell FRED pseudo source inlet conditions (see Table 1)*

Obstructed Not Confined Jet

Figure 11 and Figure 12 compare the predicted and measured centreline H_2 molar fraction:

- The CFX results capture the jet width relatively well but over-predict the concentrations. The level of over-prediction increases with increased distance from the release point.
- The FLACS simulation reproduces the concentrations well at the first downstream distance of 1.4 m but over-predicts concentrations and jet widths further downstream. Similarly, to what was obtained with CFX, the magnitude of the over-prediction increases with the distance from the release point.
- The OpenFOAM 1812 results under-predict the concentration at the first location and give excellent agreement further downstream. Again, the jet width is reproduced well in the model.
- The OpenFOAM 1912+ simulation gives good agreement with the measured jet widths but over-predicts the specific concentration quite substantially at the 4.4 m measurement location. The FRED results give the closest agreement with the measured data.
- The CFX, FLACS and OpenFOAM 1812 calculations all predict some asymmetry in the radial profiles. This is most pronounced in the FLACS modelling and is due to jet interaction with the obstacle array and the influence of gravity (measurement sensor array is on the vertical plane). An alternative option is that the geometry representation by PDR is not the most appropriate for round bars with a size similar to the mesh.

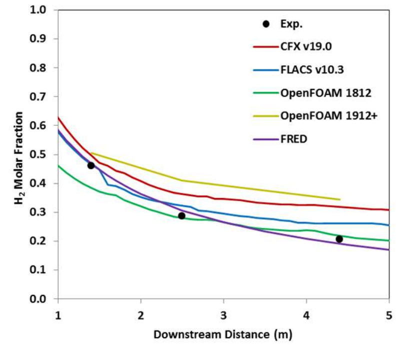

Figure 11 – Comparison of the measured and predicted centreline H_2 molar fraction for the obstructed jet

Figure 13 and Figure 14 show comparisons of the measured and predicted velocity profiles:

- The OpenFOAM 1812 calculations give centerline velocity decay in closest agreement with the measured data, whilst the other three models generally under-predict the velocity measurements.
- The CFX, FLACS and OpenFOAM 1812 all exhibit the same behavior in the predicted velocity, with the centerline decay showing drops in velocity slightly further downstream of each measurement location, which is 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. In the FLACS models, the obstacles are represented using porosities (due to the fact results are taken on a line going through the objects, they go all the way to zero), whereas in CFX and OpenFOAM 1812 the obstacles are resolved by the mesh. All the models capture the jet width relatively well, as shown by predictions of radial velocity profiles.
- The OpenFOAM 1912+ modelling gives under-prediction of the centerline velocity at measurement locations 1.4 m and 4.4 m downstream but reproduces well the measured data at 2.5 m downstream of the release point.
- The 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.

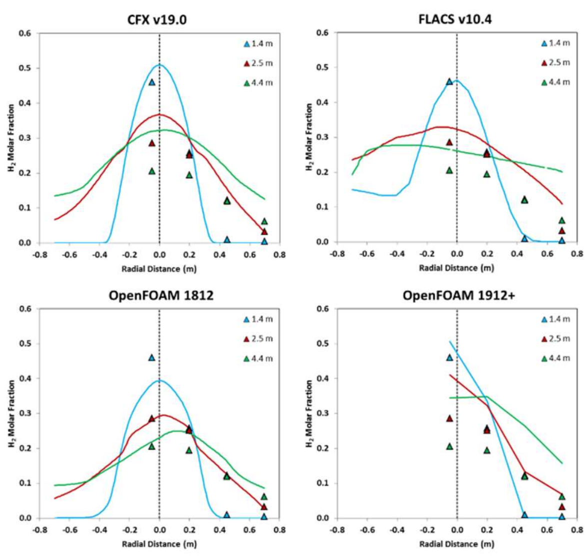

Figure 12 – Comparison of the measured (symbols) and predicted (lines) radial H2 molar fraction for the obstructed jet scenario

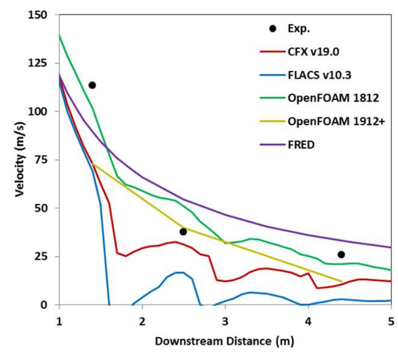

Figure 13 – Comparison of the measured and predicted centreline velocity for the obstructed jet

With regards to the turbulence field, experimental data for radial profiles of the turbulent fluctuating velocity, u' (m/s), is compared to simulation predictions, as shown in Figure 15:

- The three models (CFX, FLACS and OpenFOAM 1812) give generally similar results, with some asymmetry across the radial profiles.
- The experimental fluctuating velocity close to the jet centerline at 1.4 m is substantially lower than the predictions made using all three models. It is worth bearing in mind that the fluctuating velocity is inferred from velocity measurements in the experiments and that the level of accuracy of the data is not clear.
- The predicted values of u' at the extremities of the radial profile at 1.4 m are significantly under-predicted but are in closer agreement with the data at 2.5 m and 4.4 m.

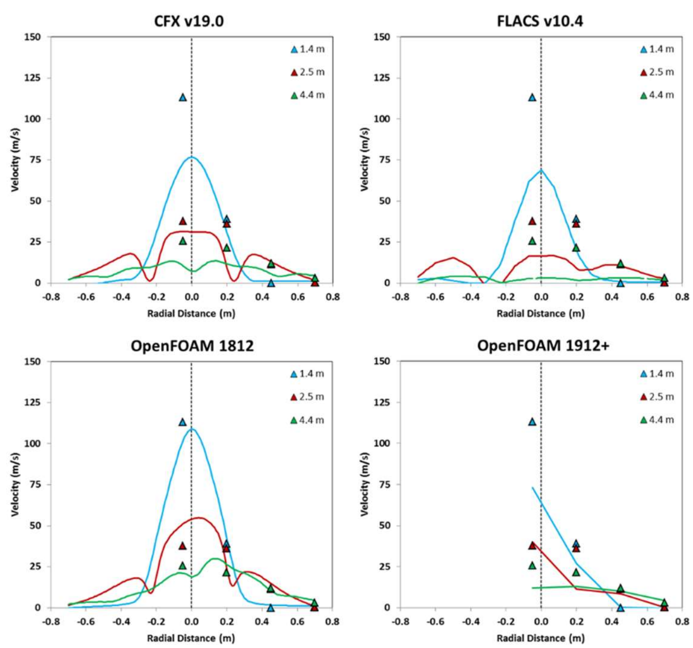

Figure 14 – Comparison of the measured (symbols) and predicted (lines) radial velocity profiles for the unobstructed jet scenario

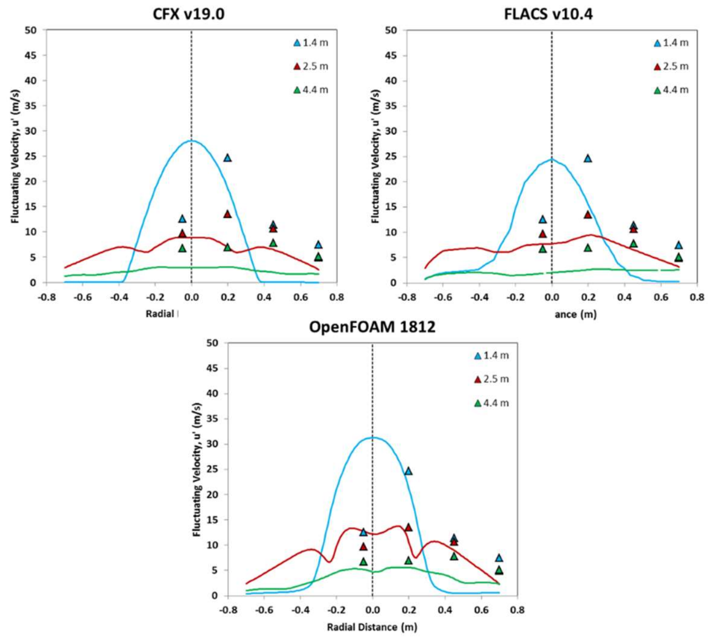

Figure 15 – Comparison of measured (symbols) and predicted (lines) radial profiles of turbulent fluctuating velocity, u'.

As was the case for the unobstructed jet, CFX has also been used with source conditions estimated using both the Ewan and Moodie (1986) approach and the Shell FRED model to simulate the obstructed jet scenario, see Figure 16. The model with the source conditions taken from FRED gives closer agreement with the measured data, similarly to the findings for the unobstructed jet case. Furthermore, the results from CFX with this source condition are comparable with those produced using OpenFOAM 1812. This indicates a good level of agreement across the two models, modelling approaches and different modellers, provided that the same source term is used.

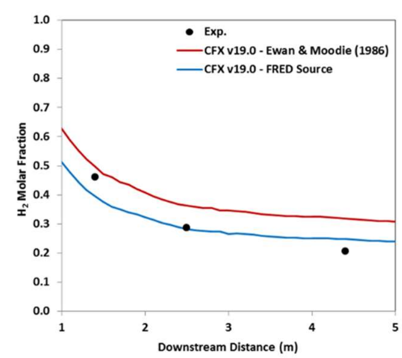

Figure 16 - Comparison of the measured centreline H_2 molar fraction for the obstructed jet to CFX v19.0 predictions using the Ewan and Moodie (1986) and Shell FRED pseudo source inlet conditions listed in Table 1

Confined Releases

Figure 17 compares the measured and prediction vertical H_2 concentration profiles for the 10.4 NL min^{-1} and 218.3 NL min^{-1} confined release scenarios, respectively. It illustrates that closer agreement between the model predictions and the measured concentrations is obtained, in general, for the higher release rate scenario. For both releases, the predicted concentrations in the transition layer, i.e. 0.6 to 0.8 m above the enclosure base, show less good agreement with the measured data for most of the models tested.

Overall, predictions of the upper layer concentration, where the H_2 concentrations are greatest, are in good agreement with the data for the 218.3 NL min^{-1} release for all the models used. However, the simulations for both versions of OpenFOAM show some over-prediction of the upper layer

concentrations for the 10.4 NL min^{-1} release. For the lower release rate scenario, the depth of the upper layer is under-predicted in the modelling using OpenFOAM 1912+ and CFX, as indicated by under-prediction of the concentration at around 0.8 m above the enclosure base.
For the purposes of further comparison, Figure 17 includes predictions of the concentration based on the approach of Linden [17], as implemented by Air Liquide [18]. This model gives predictions in good agreement with the measurements.

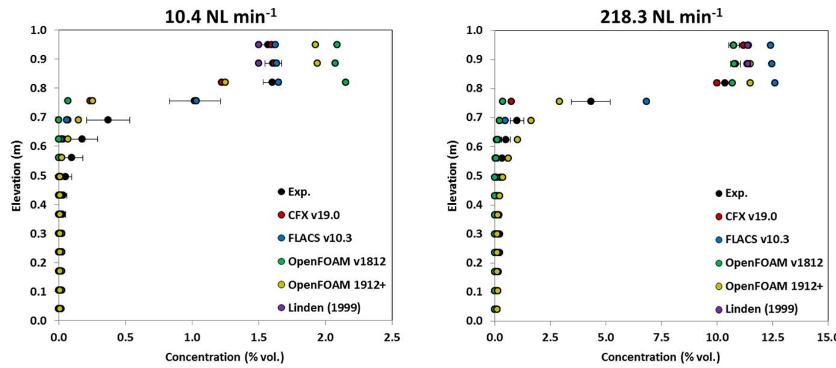

Figure 17 – Comparison of the measured and predicted H_2 concentration profiles with height inside the enclosure for the 10.4 NL min^{-1} release (on the left) and for the 218.3 NL min^{-1} release (on the right)

SUMMARY

To summarise, the model validation exercise has shown that the CFD models selected by the partners can reasonably reproduce the measured data across the selected range of scenarios considered. This helps to provide confidence that the models will produce acceptable solutions for the realistic release modelling.
Whilst the model validation results show some scatter in predictions, with both over-prediction and under-prediction of the measured data, for the purposes of the present study, the level of agreement is considered acceptable. To perform a dispersion for realistic cases it is recommended to validation versus simple cases (for instance to use 4 cases mentioned in the paper) to find out any drawback of models and find the appropriate approach before doing realistic cases. It is essential to follow this recommendation since very often consultancies tend to go direct to realistic cases without validation.
Furthermore, model predictions for realistic scenarios usually are not be compared with measured data at specific locations, instead the aim is to generate representative solutions of expected flammable cloud shapes, size and spread across the forecourt configurations. Since the model validation work is essential to show that the models are likely to be capable of achieving this successfully.
One specific outcome to note from the model validation cases involving jet releases is that the specification of the source term has been shown to be important. Results presented in this paper indicate that model predictions made with OpenFOAM 1812 and CFX are comparable when the same source conditions are used. Furthermore, using the source term from FRED gave better agreement with the measurements when used in CFX than the Ewan and Moodie [15]. For jet simulations it is recommended that a suitable jet model is used 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.

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including any opinions and/or conclusions expressed or recommendations made, do not supersede current HSE policy or guidance.

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