CFD Modelling of Underexpanded Hydrogen Jets Exiting Rectangular Shaped Openings

J.R Stewart, Senior Scientist, Health and Safety Executive, Harpur Hill, Buxton, SK17 9JN, UK

Underexpanded jet releases from circular nozzles have been studied extensively both experimentally and numerically. However, jet releases from rectangular openings have received much less attention and information on their dispersion behaviour is not as widely available. In this paper, Computational Fluid Dynamics (CFD) is used to assess the suitability of using a pseudo-source approach to model jet releases from rectangular openings. A comparative study is performed to evaluate the effect of nozzle shape on jet structure and dispersion characteristics for underexpanded hydrogen jet releases. Jet releases issuing from a circular nozzle and rectangular nozzles with aspect ratios ranging from two to eight are modelled, including resolution of the near-field behaviour. The experimental work of Ruggles and Ekoto (2012, 2014) is used as a basis for validation of the modelling approach. The CFD results show that the hazard volume and hazard distance remain largely unaffected by nozzle shape and that representing the jets using a pseudo-source approach produces conservative results for all nozzle shapes considered. This finding has useful practical implications for consequence analysis in industrial applications, such as the assessment of leaks from flanges and joins in pipework.

Keywords: Underexpanded jet, CFD, Modelling, Pseudo-source, Hydrogen, Dispersion

Introduction

As hydrogen becomes a more popular energy carrier, the number of high-pressure hydrogen process and storage systems will increase. This, together with the wide flammable range of hydrogen and low ignition energy, leads to a greater hazard potential and increased hazard analysis requirements. A scenario of particular interest is the accidental release of hydrogen. Given the high pressures typically used for hydrogen storage, i.e. 200 – 700 bar, an accidental release will usually result in the formation of a highly underexpanded jet. Whilst the study of underexpanded jet releases through circular openings is extensive, unintended releases are likely to be from non-circular holes such as cracks or punctures in pipework. Whilst existing research into hydrogen releases through non-circular holes exists, it is limited, yet nozzle shape may affect the resulting dispersion distances and flammable gas cloud volumes.

Underexpanded jets form when the ratio between the jet exit pressure, P_e, and the ambient pressure, P_a, exceeds a critical value, approximately $(P_e/P_a) > 1.8$ for natural gas and $(P_e/P_a) > 1.9$ or hydrogen. These jets are characterised by a barrel shaped expansion region at the nozzle, which culminates in a normal shock and Mach disk (Ewan and Moodie, 1986). At the exit, the jet velocity is sonic before increasing as the jet expands. The Mach disc forms at the boundary of supersonic and subsonic flow and indicates the point where the jet pressure has returned to ambient.

There is a large body of research focussed on underexpanded jets issuing from circular openings. The experimental work of Birch et al. (1984, 1987) investigating underexpanded jet structure, concentration and velocity decay in jets from circular nozzles is widely used as the basis for comparison for subsequent research into underexpanded jets. Ewan and Moodie (1986) present an experimental analysis of underexpanded jets and provide an analytical model describing velocity and concentration decay including comparison to the data of Birch et al. (1984). Their work focuses on jet releases from circular nozzles and shows that an underexpanded jet release could be represented by an equivalent sonic "pseudo-source" located at the point where the jet pressure returns to ambient, corresponding to a location just downstream of the Mach disk. The subsequent jet decay and dispersion behaviour downstream of the pseudo-source provides an accurate representation of the actual underexpanded jet (Ivings et al., 2004).

Chuech et al. (1989) present a mathematical model of underexpanded jets based on the solution to the governing equations in parabolic form to determine the jet behaviour. Their results compare favourably to a number of experimental datasets, including the data of Birch et al. (1984, 1987). A further model of underexpanded free jets is that of Cumber et al. (1995) who give a modelling approach which solves the governing equations in elliptic form. Their results reliably capture the near-field shock structure and compare well with experimental data. Birkby and Page (2001) also conduct a numerical study of underexpanded jets. Their approach incorporates a compressibility correction into their turbulence model in an attempt to gain greater accuracy in capturing the shocks near to the nozzle.

Ivings et al. (2010) use a pseudo-source approach within a Computational Fluid Dynamics (CFD) model of jet releases from circular openings in ventilated enclosures. The use of a pseudo-source approach to represent an underexpanded jet within a CFD model is common and Papanikolaou et al. (2012) provide a review of different approaches. If gas dispersion, rather than near-field jet structure, is of primary interest then a pseudo-source representation of the jet is often used. This can significantly reduce the computational cost of the CFD model, as a much coarser mesh can be used when the strong pressure, temperature and velocity gradients associated with the presence of shocks is ignored. Hall et al. (2015) present experimental and numerical modelling of high-pressure hydrogen releases from circular nozzles. The numerical model uses a utility program to calculate a pseudo-source based on the isentropic expansion of gas from the reservoir to the nozzle, in much the same manner as the approach described by Ewan and Moodie (1986).

The work of Ewan and Moodie (1986) is widely used but their method focusses on jet releases from circular nozzles. One question, which this paper seeks to address, is whether high-pressure jet releases from non-circular holes can be adequately modelled using a pseudo-source approach. This has implications for industrial applications, since it is likely that an accidental release will be through a non-circular orifice. If the pseudo-source approach gives comparable dispersion results to those for jets exiting rectangular openings, then this would give confidence in the methodology that is typically used for consequence modelling in industrial risk assessments.

A number of studies have investigated underexpanded jets from non-circular holes. The experimental work conducted by Wakes et al. (2002) investigates the influence of orifice shape for jets from high aspect ratio, curved flange orifices. Wakes (2003) also conducts numerical simulations of high-aspect ratio cross-sectional jets to compare the behaviour of jets issuing from both curved and planar slot orifices. Holdø and Simpson (2002) present modelling of rectangular slot jets to investigate the importance of the jet boundary condition. Makarov and Molkov (2010) present numerical modelling results of an underexpanded hydrogen jet exiting a large aspect ratio rectangular nozzle. Their findings show that, from a safety perspective, there is practically no difference between the behaviour of their rectangular jet and an equivalent round jet in the far field. This indicates that a pseudo-source approach should adequately represent an underexpanded jet issuing from a rectangular nozzle if the hazard distance and volume are of primary interest. Ruggles and Ekoto (2012, 2014) present experimental studies into the impact of nozzle geometry on the behaviour of underexpanded hydrogen jet releases. Their work compares the behaviour of a number of jets issuing from rectangular nozzles with aspect ratios 2, 4 and 8 with a circular jet. Their work focusses on the near-field jet behaviour.

This paper describes CFD modelling work conducted by the Health and Safety Executive as part of the Hydrogen and Fuel Cell (H2FC) European Infrastructure project. The modelling is used to assess the suitability of using a pseudo-source approach to model releases from rectangular openings and to investigate the impact of nozzle shape on hydrogen dispersion from underexpanded jet releases. The experimental work of Ruggles and Ekoto (2012, 2014) is used as a basis for validation of the modelling approach. Emphasis is placed on the comparison of the hazard distances and flammable volumes for hydrogen jets issuing from circular and rectangular nozzles with equivalent mass flow rates and release areas. The rectangular nozzles have aspect ratios ranging from 2 to 8. The jets are modelled using two approaches for the near-field flow. In the first approach, the near-field behaviour is fully resolved, using a fine mesh. In the second, the pseudo-source approach of Ewan and Moodie (1986) is used.

CFD Modelling

CFD Modelling Approach

The general-purpose CFD code ANSYS CFX 16.0 (2015) is used to model horizontally oriented underexpanded hydrogen jets with a stagnation-to-ambient pressure ratio of around 10:1, following the experimental work of Ruggles and Ekoto (2012). A mean reservoir pressure of 9.83 bar(a) gives a jet release with pressure of 5.15 bar(a), temperature of 244.8 K and velocity of 1203 m/s at the nozzle exit. The modelled hydrogen jet discharged into air with ambient pressure and temperature of 0.98 bar(a) and 296 K, respectively. The base case, which is used for model validation, involves a circular nozzle with a diameter of 1.5 mm (Ruggles and Ekoto, 2012). Three rectangular nozzle configurations with aspect ratios of 2, 4 and 8 are also modelled to investigate the effects of nozzle shape. The dimensions of each non-circular nozzle are selected to ensure an equivalent nozzle area and modelled mass flow rate as for the circular nozzle case.

All of the modelled jets are simulated directly from the nozzle exit in three-dimensions (3D). Due to the large variation in timescales between the grid-cell residence time near the nozzle and that further downstream, a two-stage simulation approach is adopted to avoid numerical instabilities. For the first stage, the flow is simulated from the nozzle exit to a point 0.25 m downstream. This particular domain size is chosen to coincide with the experimental measurements of Ruggles and Ekoto (2012), which are used to validate the CFD model. For the second stage, the flow from 0.25 m downstream of the nozzle to a distance of 3.5 m downstream of the nozzle was simulated with the downstream boundary data from stage one imposed as an inflow condition for stage two of the model.

The first stage of the simulations uses a domain size of 0.25 m × 0.1 m × 0.1 m; the domain size for the second stage simulation is 3.25 m × 1 m × 1 m. For both stages, the upstream domain boundary has a 0.5 m/s co-flow boundary condition imposed to prevent numerical instabilities due to introducing a high-speed jet into stagnant surroundings. The initial flow in the domain is set to 0.5 m/s along the jet axis for the same reason. The remaining domain boundaries are assigned fixed-pressure entrainment boundaries at ambient pressure.

The hydrogen distribution is modelled using a multi-component flow approach in which the hydrogen mass fraction is modelled using a scalar transport equation (ANSYS, 2015). Buoyancy is active in the model. However, in comparison to the momentum of the jet, the influence of buoyancy is negligible, particularly in the near-field.

Turbulence is modelled using the standard $k - \varepsilon$ model following best practice guidelines for simulating highly underexpanded jets (ERCOFTAC, 2011). Sensitivity to the choice of turbulence model and the inclusion of a compressibility correction (Sarkar et al., 1991) are investigated by comparison with the experimental data of Ruggles and Ekoto (2012), the results of which are presented in Section 2.3. Heat transfer is modelled using the ANSYS CFX Total Energy formulation and the High Speed Numerics option is used to aid numerical stability of the solver when dealing with compressible flow (ANSYS, 2015).

The computational mesh comprised tetrahedral cells with refinement in the region of the nozzle and gradual expansion axially downstream. Sensitivity to the computational mesh is investigated by varying the grid resolution for both the first and second simulation stages to produce a matrix of nine grid sensitivity simulations. The results presented in this paper are calculated using grid sizes of 0.3 million and 0.33 million nodes for a full 3D representation of the jet for stages one and two respectively, with the jet inlet boundary resolved using approximately 150-170 nodes, depending on the nozzle shape.

CFD Modelling Validation

The CFD modelling approach described above was used to simulate the experiments conducted by Ruggles and Ekoto (2012, 2014). The modelling approach has been validated against their underexpanded round jet data. The primary quantity of interest for comparison between the model and the experiment was the axial hydrogen concentration decay within the jet. The hazard distance and flammable volume, taken as the distance to half the lower flammable limit (LFL) of hydrogen (i.e. 2% v/v) and the volume of gas above ½ LFL, from the two-stage model were compared to values given by the H2FC FreeJet tool (HSL, 2016a) and the Quadvent 2 software package (HSL, 2016b). FreeJet is an integral model that determines axial concentration decay from jet releases using a combination of a pseudo-source and a Gaussian jet model based on the correlation of Chen and Rodi (1980). Quadvent 2 is a model for predicting gas cloud volumes for hazardous area classification. The model is based on the work of Webber et al. (2011) and is developed by the Health and Safety Laboratory. The pseudo-source is calculated assuming isentropic expansion from storage conditions to the nozzle exit, similarly to the Ewan and Moodie (1986) approach.

The model validation included a grid sensitivity analysis to assess the impact of mesh resolution on the predicted axial concentration decay, Mach disk size and location. Coarse, medium and fine grid resolutions were used, corresponding to 0.3, 1.0 and 3.8 million nodes for the full 3D, near-field model and approximately 150, 360 and 560 nodes to resolve the jet inlet boundary, respectively.

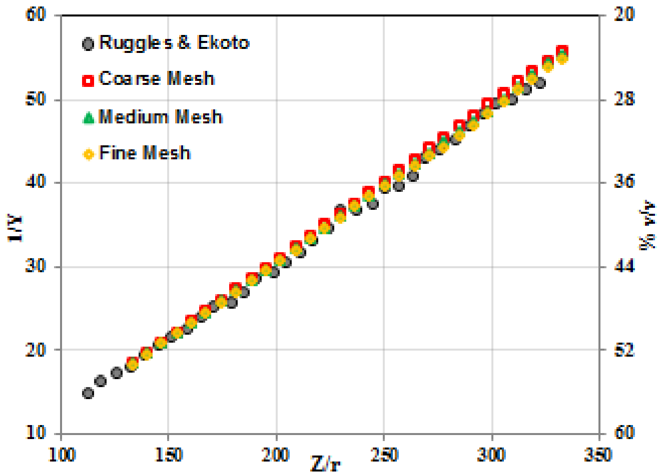

Figure 1 Comparison of the experimental (Ruggles and Ekoto, 2012) and CFD results for the inverse hydrogen mass fraction against normalised axial distance

Figure 1 shows the inverse hydrogen mass fraction, 1/Y, along the jet axis, Z, normalised by the nozzle radius, r, for the Ruggles and Ekoto (2012) round jet and the corresponding CFD results. The CFD model results match the experimental data well with little variation across the three grid resolutions used. The largest variation in the predicted hydrogen concentration between meshes was found to be 0.5% (v/v).

Whilst the mesh choice had little impact on the concentration decay for the model of the Ruggles and Ekoto (2012) underexpanded round jet, the influence of the mesh on predicting the Mach disk location is much greater. Figure 2 shows a comparison of the barrel shock region for each of the three mesh resolutions used. The measured Mach disk diameter was 1.3 mm, located 3.05 mm (Z/r ≈ 4) downstream of the nozzle. The solid black lines within Figure 2 show these measurements.

Figure 2 clearly shows that increasing the mesh resolution results in a more accurate representation of the barrel shock region. In addition, a finer mesh results in a more well-defined and precisely captured Mach disk size and location, although the differences between the results on the medium and fine meshes are small. The axial hydrogen concentration is, in this case, independent of the grid resolution. This indicates that modelling underexpanded jets directly from the nozzle need not be as computationally expensive as is sometimes assumed, at least in terms of obtaining the correct concentration distribution.

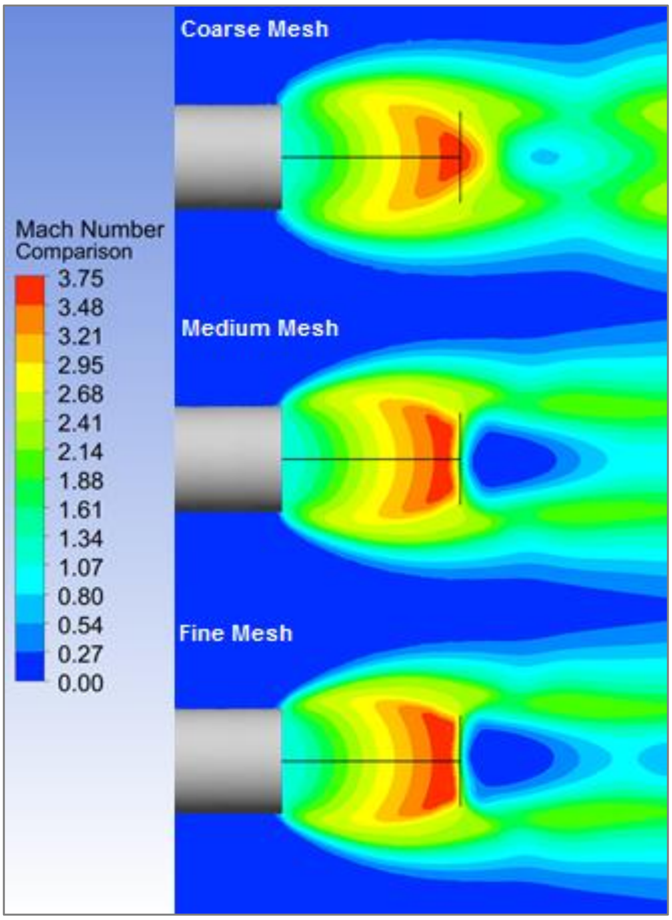

Figure 2 Comparison of barrel shock region and Mach disk resolution for different computational meshes

To assess the model predictions of hazard distance and flammable volume, the first stage simulation conditions at the downstream boundary were imposed as an inlet condition for a far-field dispersion simulation. The volumes of gas above ½ LFL from each simulation stage were summed to give a single hazard volume for comparison to the H2FC FreeJet and Quadvent 2 (HSL, 2016a,b) predictions. The sensitivity to mesh resolution was assessed based on simulations using approximately 0.3, 1.0 and 3.2 million nodes for the second simulation stage with inlet conditions taken from each of the three first stage simulation results. The resulting matrix of simulations gave flammable volumes ranging from 0.141 m3 to 0.156 m3, and hazard distances ranging from 2.73 m to 2.75 m ($Z/r \approx 3640$ to 3666). The H2FC FreeJet predictions gave a hazard distance of 3.36 m and a hazard volume of 0.210 m3, compared to a hazard distance of 2.78 m and a hazard volume of 0.277 m3 as predicted by Quadvent 2 (version 2.0.0.15). The results show that the CFD model predicts smaller gas cloud volumes and hazard distances than both the H2FC FreeJet and Quadvent 2 models.

The CFD modelling approach used to simulate an underexpanded hydrogen jet release through a circular nozzle has been shown to give excellent agreement with experimental data in the near field (Ruggles and Ekoto, 2012). Furthermore, the model gives hazard volume and distance predictions well within a factor of two of those obtained with the H2FC FreeJet and Quadvent 2 models. A key uncertainty is that the experimental data does not extend far enough downstream to be able to assess how well the model predicts the distance to ½ LFL. However, given that the primary interest of this paper is to assess the relative differences in dispersion behaviour between underexpanded jet releases from different nozzle shapes, the level of accuracy shown by the model in the near field and the comparative performance of the CFD model with other jet models is deemed adequate for the purposes of this study.

Sensitivity Studies

Further to the grid sensitivity analysis described above, additional CFD simulations were undertaken to assess the sensitivity to the choice of turbulence model, turbulence intensity of the jet source and magnitude of the co-flow velocity at the upstream domain boundary.

The ERCOFTAC QNET Best Practice Guidelines (ERCOFTAC, 2011) suggest that the standard $k - \varepsilon$ turbulence model performs as well as a Sarkar-corrected (Sarkar et al., 1991) or a basic Reynold's stress turbulence model for resolving shock structure in highly underexpanded jets. However, the $k - \varepsilon$ model has a tendency to over-predict diffusion in turbulent jets, leading to increased spreading and faster axial concentration decay. As such, the sensitivity of the CFD model to the choice of turbulence model has been investigated using the ANSYS CFX 16.0 formulations (ANSYS, 2015) of the standard $k - \varepsilon$ model and the widely-used SST model, together with two versions of the $k - \varepsilon$ model modified to account for over-prediction of diffusion and jet spreading. The first of these encompasses the correction proposed by Sarkar et al. (1991) the second uses the modification proposed by Pope (1978), as further discussed by Smith et al. (2004), where the turbulence model parameter $C_{\varepsilon 1}$ is adjusted from the standard value of 1.44 to a modified value of 1.60 to reduce the over-prediction of jet spreading by the standard $k-\varepsilon$ model.

Figure 3 shows the near-field axial hydrogen concentration decay for the four turbulence models along with the experimental data (Ruggles and Ekoto, 2012). It is clear that the standard $k-\varepsilon$ model most closely matches the experimental data and the SST model gives similar, though slightly under-predicted, results. The Sarkar and Pope corrected $k-\varepsilon$ variants give markedly different results to the experimental data with large over-predictions of the axial hydrogen concentration and greater rates of concentration decay, particularly for the diffusion corrected (Pope, 1978; Smith et al., 2004) model. At 0.1 m downstream of the nozzle, the Sarkar et al. (1991) and Pope (1978) corrected $k-\varepsilon$ variants give hydrogen concentrations approximately 58% and 81% greater than the standard $k-\varepsilon$ model respectively. At 0.25 m downstream of the nozzle, the corresponding differences are approximately 19% and 58% for the Sarkar and Pope corrected models respectively. This result illustrates that both the Sarkar et al. and the Pope corrections, in this case, give significantly higher predicted axial hydrogen concentration and greater rates of concentration decay along the jet centreline than the standard $k-\varepsilon$ turbulence model.

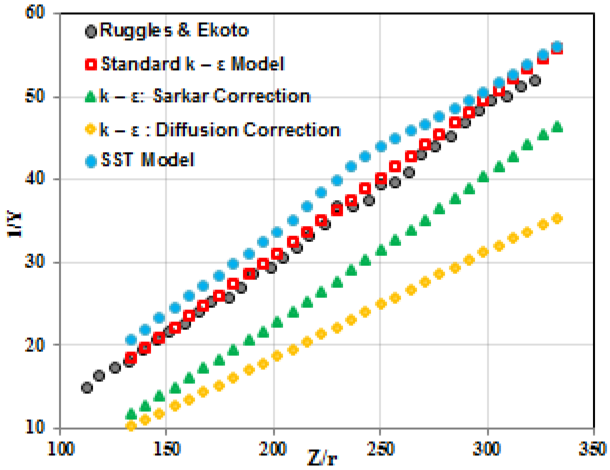

Figure 3 Comparison of the experimental (Ruggles and Ekoto, 2012) and CFD turbulence model sensitivity results for the hydrogen concentration against the axial distance

A further comparison of the standard $k-\varepsilon$ model results with those for the model using the Sarkar et al. (1991) correction shows that the reduction in jet spreading for the latter model gives a significantly reduced hazard volume of 0.112 m^3, compared with the 0.153 m^3 obtained for the standard $k-\varepsilon$ model. However, the predicted hazard distance slightly increases, by about 1%, when the Sarkar et al. (1991) correction is used. The model with the Sarkar et al. (1991) correction predicts a longer but thinner hydrogen cloud as compared to predictions made using the standard $k-\varepsilon$ model.

Whilst the $k-\varepsilon$ turbulence model has been shown to give good agreement with experimental data for the circular jet, the anisotropy present for the rectangular, slot jet releases raises questions about the applicability of this turbulence model for this application. However, the work presented here is intended to be a pragmatic study of the influence of nozzle shape, rather than a detailed turbulence modelling study and as such, validating the choice of turbulence model for plane and slot jets is considered a topic for future work.

Model sensitivity to the turbulence intensity of the jet source was investigated using values of 1%, 5% and 10% at the jet inlet. The three cases gave a variation in the hazard distance predictions of less than 5×10^{-4} m^3, or less than 0.25% difference in relative terms, and gave the same predicted hazard distance, to within 1 cm.

The sensitivity of the model predictions to the magnitude of the co-flow velocity at the upstream domain boundary was examined using imposed co-flow velocities of 0.1 m/s, 0.25 m/s and 0.5 m/s, for both the near and far-field simulation stages. The results showed little sensitivity to the choice of co-flow velocity, with a variation in the predicted flammable volume and hazard distance of less than 5% and 1.5%, respectively, across the three conditions used.

Overall, it can be concluded from these sensitivity analyses that the influence of jet turbulence intensity and co-flow velocity magnitude on the hazard distance and volume is small. The impact of the choice of turbulence model is more pronounced and it is therefore important to select an appropriate turbulence model for the scenario being simulated. For the present work the standard $k-\varepsilon$ turbulence model gives the results in closest agreement with the experimental data and it is also consistent with the recommendations made in the ERCOFTAC QNET Best Practice Guidelines (ERCOFTAC, 2011) for modelling highly-underexpanded jets

Results

One of the aims of this paper was to assess the impact of nozzle shape on hydrogen dispersion from underexpanded jet releases. To do this, CFD modelling has been used to compare the hazard distance, the flammable volume and the axial hydrogen concentration decay for jets issuing from a 1.5 mm diameter circular nozzle and rectangular openings with aspect ratios of 2, 4 and 8.

The CFD results show that the nozzle shape has a significant impact on the flow field within the immediate vicinity of the nozzle. For the jets exiting rectangular openings, axis-switching behaviour was observed, whereby the jet plume undergoes a ninety-degree rotation such that the minor and major axes of the nozzle are switched. This behaviour results in the formation of an asymmetric jet that is wider across the minor axis than the major axis of the nozzle. This behaviour is consistent with the experimental work of Zaman (1995) and the numerical analysis of a large aspect ratio rectangular hydrogen jet release by Makarov and Molkov (2010). Figure 4 illustrates the predicted axis switching behaviour for the jets from each of the nozzles considered. As the aspect ratio of the nozzle is increased, the downstream extent of the jet core, in which the concentration is above the upper flammability limit of hydrogen (74% v/v), is reduced. Figure 4 also shows that this core region increases in width across the nozzle minor axis and reduces in width across the nozzle major axis with increasing nozzle aspect ratio. The round jet exhibits axisymmetric behaviour and has a core length that is larger than for any of the rectangular nozzle jets considered.

Figure 5 shows radial hydrogen concentration profiles across the nozzle minor axis for the four considered nozzle shapes at a distance of 0.03 m (Z/r = 40) downstream of the opening. This figure clearly demonstrates that the plume width increases and the centreline hydrogen concentration decreases with increased nozzle aspect ratio, consistent with the findings shown in Figure 4.

Figure 6 shows the centreline axial hydrogen concentration decay for the four jets considered. This figure shows that in the region 0.025 m (Z/r = 33) to 0.175 m (Z/r = 233) downstream of the opening there is only a marginal difference in the results for the different nozzle shapes used. Beyond this distance, the results are almost identical for all of the considered nozzle shapes.

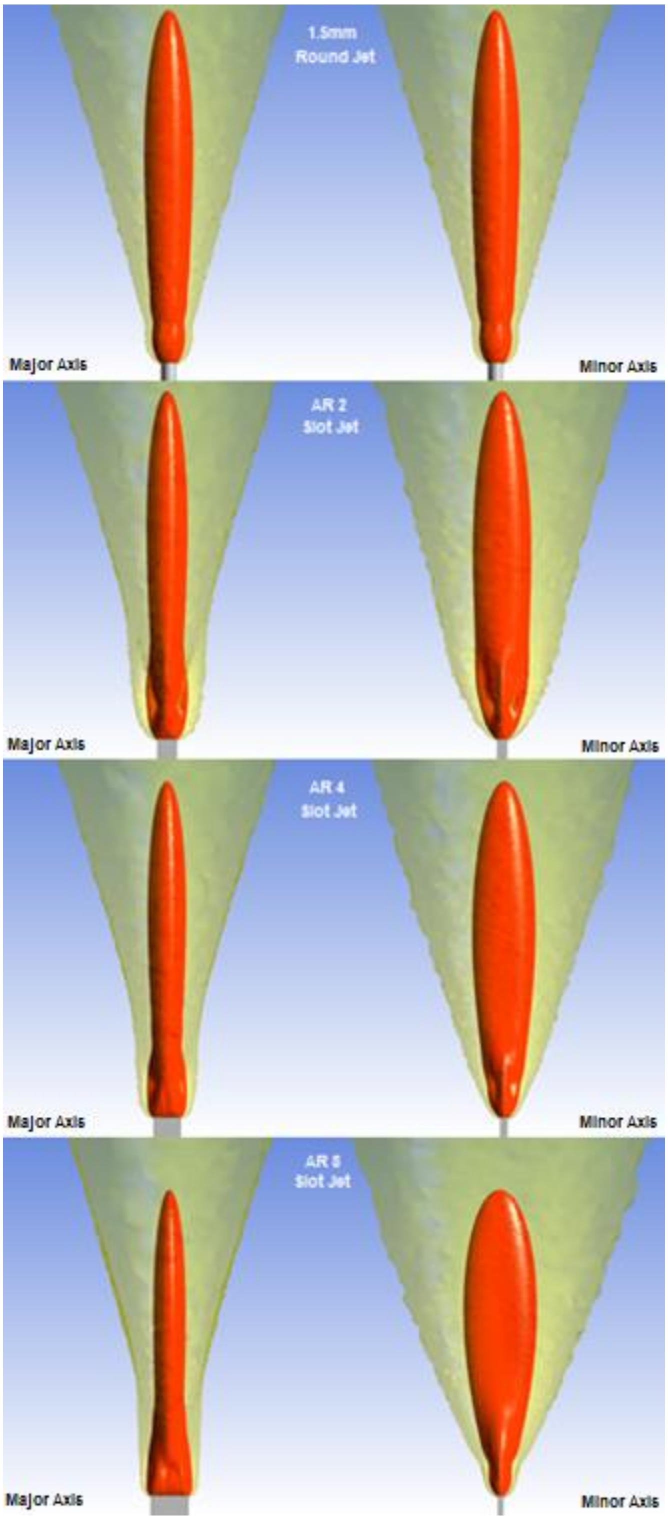

Figure 4 Isosurfaces at the lower and upper flammability limits of hydrogen, yellow (2% v/v) and red (74% v/v) respectively, for the considered nozzle shapes. From top to bottom: round jet, rectangular nozzle aspect ratio = 2, 4 and 8

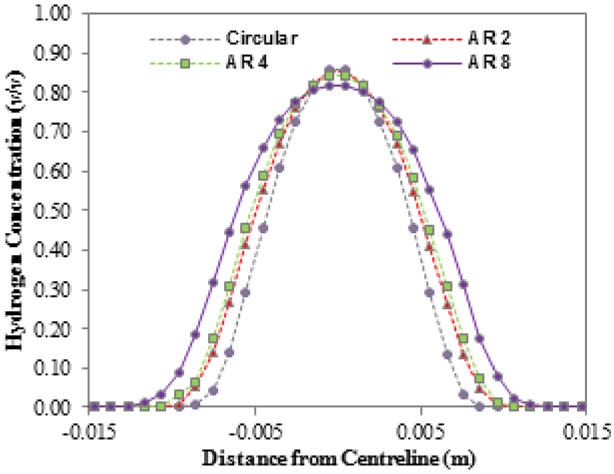

Figure 5 Radial hydrogen concentration profiles across the nozzle minor axis for the four considered nozzle shapes at a distance of 0.03 m downstream of the nozzle. Here AR 2, 4 and 8 represent rectangular nozzles with aspect ratio = 2, 4 and 8 respectively

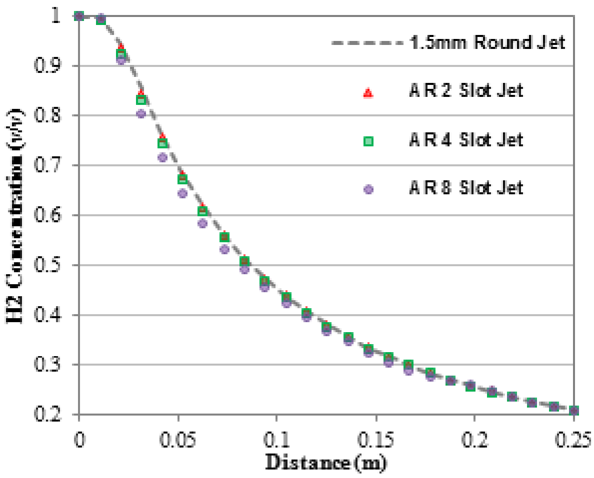

Figure 6 Centreline axial hydrogen concentration profiles for the four considered nozzle shapes

Beyond 0.175 m, all four nozzle shapes give approximately the same axial concentration profiles to the downstream domain boundary (of the near-field simulation) at 0.25 m (Z/r = 333). This result indicates that the behaviour of underexpanded hydrogen jet releases through rectangular openings approximates that of a circular nozzle release at larger distances downstream of the nozzle.

Comparing the hazard distance predictions for the four nozzles considered shows that nozzle shape has little impact on the distance to ½ LFL. For the circular nozzle, the predicted hazard distance was 2.73 m. For all three rectangular nozzles, the predicted hazard distance was 2.72 m, a difference of less than 0.5% from the circular nozzle result.

A slightly larger variation in the predicted hazard volume was seen amongst the different nozzle shapes. The predicted values ranged from 0.150 m^3 to 0.152 m^3 across the rectangular nozzle jets, with the smallest volume given by the nozzle with an aspect ratio of four. Comparison to the hazard volume of 0.153 m^3 predicted for the round jet produces a maximum difference due to nozzle shape of less than 2.5% in relative terms.

A CFD simulation was also undertaken in which the jet was modelled using a pseudo-source instead of resolving the near source behaviour. The pseudo-source was defined using the approach of Ewan and Moodie (1986). The Ruggles and Ekoto (2012) round jet was represented by a source 3.5 mm downstream of the nozzle with a diameter of 3.4 mm, a velocity of 1194 m/s and a temperature of 245.2 K.

For consistency, the same two-stage CFD modelling approach was used to simulate the hydrogen jet. The CFD model based on the pseudo-source approach gives a predicted hazard distance of 3.18 m and a hazard volume of 0.281 m^3, a 16.5% and an 83.4% increase from the resolved circular nozzle results respectively. From these results, it is evident that the pseudo-source approach is more conservative than a resolved-nozzle modelling approach for the Ruggles and Ekoto (2012) underexpanded hydrogen jet release. Given that the results for the jets exiting the rectangular openings approximate those for the circular nozzle in terms of hazard distance and volume, it follows that the pseudo-source approach is also more conservative than a resolved-nozzle approach for the slot jets considered here.

Conclusions

This paper has considered the effect of nozzle shape on hydrogen dispersion from underexpanded jet releases. The aim of the work was to assess the suitability of using a pseudo-source modelling approach to simulate jet releases from non-circular openings and to compare the dispersion behaviour of releases from circular and rectangular openings with different aspect ratios. The main quantities of interest were the axial hydrogen concentration, the flammable volume and the hazard distance, based on the ½ LFL concentration of hydrogen (2% v/v).

Using a Ewan and Moodie (1986) pseudo-source within the CFD model to avoid simulating the near-field jet behaviour has been shown to give conservative results for the hazard volume and distance for all of the considered releases. Predictions of the hazard distance and hazard volume are more than 15% and 80% greater, respectively, when a pseudo-source model is used as compared to a resolved-nozzle modelling approach. As such, adopting a pseudo-source modelling approach for underexpanded jets from non-circular openings would be adequate from a safety analysis perspective. This suggests that for real leak scenarios, in which the nozzle geometry is unknown, it is reasonable to use a model based on a pseudo-source approach.

The results of the CFD study have shown that, for the releases considered, nozzle shape has a negligible effect on the resulting hazard quantities for underexpanded hydrogen releases despite the flow structure in the immediate vicinity of the nozzle being very different for rectangular and circular openings. For the former, rotational behaviour of the jet results in axis switching, bringing about a 90° rotation of the jet such that the hydrogen plume is wider across the minor axis than the major axis of the opening. Releases from circular nozzles do not exhibit this behaviour.

The axial hydrogen concentration was shown to be slightly lower for the rectangular openings than the circular nozzle in the region approximately 16 to 117 diameters downstream of the nozzle. The difference between the circular and rectangular nozzle axial hydrogen concentrations in this region increased with increasing nozzle aspect ratio. Beyond 117 nozzle diameters downstream of the opening, all of the rectangular jets showed axisymmetric behaviour.

For the case of the circular opening, increasing the mesh resolution in the near field resulted in a more clearly resolved barrel shock region. Furthermore, the predicted Mach disk size and location more accurately matched the experimental results the finer the computational mesh. However, the choice of mesh had negligible impact on the CFD predicted axial hydrogen concentration decay. This indicates that if far-field dispersion characteristics are of primary interest, underexpanded releases can be simulated with relatively coarse meshes near the nozzle, if a pseudo-source will not be used.

The work described in this paper focussed on a single set of release conditions for an underexpanded hydrogen jet issuing through four different nozzle shapes. Expanding on the scope of this paper to include the study of hydrogen jets at higher nozzle-exit-to-ambient pressure ratios, representative of those used for hydrogen storage vessels, would be a useful next step. Furthermore, repeating the work for an increased range of nozzle aspect ratios would help to provide a more comprehensive understanding of hydrogen dispersion behaviour from underexpanded jets issuing from rectangular openings. A more extensive turbulence modelling study in which the CFD modelling approach is validated for jet releases from plane and slot nozzles could also be performed to provide further confidence in the modelling results for non-circular jets.

Aside from carrying out further work to investigate the implications of nozzle shape and exit pressure for hydrogen releases, it would be of interest to undertake similar work for other gases. The expectation is that other gases will behave similarly to hydrogen and that assuming a circular nozzle, or using a pseudo-source representation, would provide conservative dispersion predictions.

Acknowledgments and Disclaimer

The work described in this paper was undertaken as part of the H2FC Integrating European Infrastructure project, with co-funding from the Health and Safety Executive (HSE) and the European Commission (Grant No. 287855). The contents of the publication, including any opinions and/or conclusions expressed, are those of the author alone and do not necessarily reflect HSE policy.

The author would also like to thank Mat Ivings, James Hoyes and Simon Gant (HSE) for their input, comments and advice.

References

ANSYS, 2015. ANSYS CFX Solver Theory Guide Release 16, ANSYS Inc., January 2015.

Birch, A.D., Brown, D.R., Dodson, M.G., Swaffield, F., 1984. The structure and concentration decay of high pressure jets of natural gas. Combustion Science and Technology. 36, 249-261.

Birch, A.D., Hughes, D.J., Swaffield, F., 1987. Velocity decay of high pressure jets. Combustion Science and Technology. 52, 161-171.

Birkby, P., Page, G.J., 2001. Numerical predictions of turbulent underexpanded sonic jets using a pressure-based methodology. Proceedings of the Institute of Mechanical Engineers, Part G: Journal of Aerospace Engineering. 215 (3), 165-173.

Chen, C. J., Rodi, W., 1980. Vertical turbulent buoyant jets: a review of experimental data. HMT - Science and Applications of Heat and Mass Transfer, Vol.4

Chuech, S.G. Lai, M.C., Faeth, G.M., 1989. Structure of turbulent sonic underexpanded free jets. AIAA Journal. 27 (5), 549-559.

Cumber, P.S., Fairweather, M., Falle, S.A.E.G., Giddings, J.R., 1995. Structure of turbulent, highly underexpanded jets. Journal of Fluids Engineering. 117 (4), 599-604.

ERCOFTAC, 2011. ERCOFTAC QNET – CFD Wiki: Underexpanded Jet.http://qnet-ercoftac.cfms.org.uk/w/index.php/Underexpanded_jet (accessed 20/02/16).

Ewan, B.C.R., Moodie, K., 1986. Structure and velocity measurements in underexpanded jets. Combustion Science and Technology. 45 (5-6), 275-288.

Hall, J., Hooker, P., O'Sullivan, L., Angers, B., Hourri, A., Bernard, P., 2015. Flammability profiles associated with high-pressure hydrogen jets released in close proximity to surfaces. ICHS 2015L 6th International Conference for Hydrogen Safety, Yokohama, Japan, 19-21 October 2015.

Holdø, A.E., Simpson, B.A.F., 2002. Simulations of high-aspect-ratio jets. International Journal for Numerical Methods in Fluids. 39, 343-359.

Health and Safety Laboratory (HSL), 2016a. H2FC Sage Framework - Free Jet Model. http://www.h2fc.eu/sageserver.html (accessed 16/11/16)

Health and Safety Laboratory (HSL), 2016b. Quadvent 2 http://www.hsl.gov.uk/products/quadvent-2 (accessed 16.11.16)

Ivings, M.J, Lea, C.J, Ledin, H.S, Pritchard, D.K, Santon, R., Saunders, C.J., 2004. Outstanding safety questions concerning the use of gas turbines for power generation – Executive Report. Health and Safety Laboratory Report CM/04/02.

Ivings, M.J., Gant, S.E., Saunders, C.J., Pocock, D.J., 2010. Flammable gas cloud build up in a ventilated enclosure. Journal of Hazardous Materials. 184, 170-176.

Makarov, D., Molkov, V., 2010. Structure and concentration decay in supercritical plane hydrogen jet. 8th International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions, Keio University, Yokohama, Japan.

Papanikolaou, E., Baraldi, D., Kuznetsov, M., Venetsanos, A., 2012. Evaluation of notional nozzle approaches for CFD simulations of free-shear under-expanded hydrogen jets. International Journal of Hydrogen Energy. 37(23), 18563-18574.

Pope, S. B., 1978. An explanation of the turbulent round-jet/plane-jet anomaly. AIIA Journal, 16 (3), pp. 279-281.

Ruggles, A.J., Ekoto, I.W., 2012. Ignitability and mixing of underexpanded hydrogen jets. International Journal of Hydrogen Energy. 37(22), 17549 – 17560.

Ruggles, A.J., Ekoto, I.W., 2014. Experimental investigation of nozzle aspect ratio effects on underexpanded hydrogen jet release characteristics. International Journal of Hydrogen Energy. 39, 20331-20338.

Sarkar, S., Erlebacher, G., Hussaini, M.Y., Kreiss, H.O., 1991. The analysis and modelling of dilatational terms in compressible turbulence. Journal of Fluid Mechanics. 227, 473-493.

Smith, E.J., Mi, J., Nathan, G. J., Dally, B. B., 2004. Preliminary examination of a "Round jet initial condition anomaly" for the k-ε turbulence model. 15th Australasian Fluid Mechanics Conference, The University of Sydney, Sydney, Australia, 13-17 December 2004. http://web.aeromech.usyd.edu.au/15afmc/proceedings/papers/AFMC00083.pdf.

Wakes, S.J., Holdø, A.E., Meares, A.J., 2002. Experimental investigation of the effect orifice shape and fluid pressure has on high aspect ratio cross-sectional jet behaviour. Journal of Hazardous Materials. A89, 1-27.

Wakes, S.J., 2003. Computational fluid dynamic modelling of high aspect ratio cross-sectional jets I: The effect of orifice shape on jet behaviour. ASME 2003 Pressure Vessels and Piping Conference, Cleveland, Ohio, USA, 20-24 July 2003.

Webber, D., Ivings, M.J., Santon, R.C., 2011. Ventilation theory and dispersion modelling applied to hazardous area classification. Journal of Loss Prevention in the Process Industries. 24, 612-621.

Zaman, K. B. M. Q., 1995. Axis switching and spreading of an asymmetric jet – the role of vorticity dynamics. 33rd Aerospace Science Meeting and Exhibit, Reno, Nevada, USA, January.