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CFD Modelling of Underexpanded Hydrogen Jets Exiting Rectangular Shaped Openings

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Contents

Overview

Overview & Aims

- This paper describes CFD modelling conducted by HSE as part of the Hydrogen and Fuel Cell (H2FC) European Infrastructure project
- Primary aims of the work were:
  - to assess the use of a pseudo-source to model jets from non-circular openings
  - to consider the impact of nozzle shape on H_2 dispersion from underexpanded jets
- H_2 jets from circular and rectangular nozzles with aspect ratios of 2, 4 and 8 were considered

Overview & Aims

- Round jet data of Ruggles & Ekoto (2012) was used to validate the CFD modelling
- Remainder of the study considers comparative behaviour of jets from different nozzles:
  - Flammable volume (taken as the volume with ½ LFL < $conc^{\underline{n}}$ < UFL)
  - Hazard distance (downstream distance to ½ LFL)
- Hazard quantity predictions from the CFD model were also compared to tools produced by HSE:
  - Quadvent 2.0 (HSL, 2016a)
  - H2FC FreeJet (HSL, 2016b)

CFD Modelling Approach

CFD Modelling Approach – Overview

- ANSYS CFX 16.0 (2015) was used for this study
- Hydrogen jets with a stagnation-to-ambient pressure ratio of 10:1 were modelled
- Jet releases were simulated directly from the orifice in 3D:
  - 1.5 mm circular orifice (base case)
  - Rectangular openings with AR=2, 4 & 8
- A two-stage approach was used in the modelling due to large differences in cell residence time
- A pseudo source model was also used

CFD Modelling Approach – Jet Source

- The round jet base case was modelled using the conditions given by Ruggles & Ekoto (2012)
- The rectangular orifice cases were modelled with the same mass flow rate and cross-sectional area as the base case

	Ambient	Stagnation	Nozzle Exit
Pressure (kPa)	98.37	983.20	515.40
Temperature (K)	296.0	295.4	244.8
Velocity (m/s)	N/A	N/A	1202.7

Ruggles & Ekoto (2012) Data

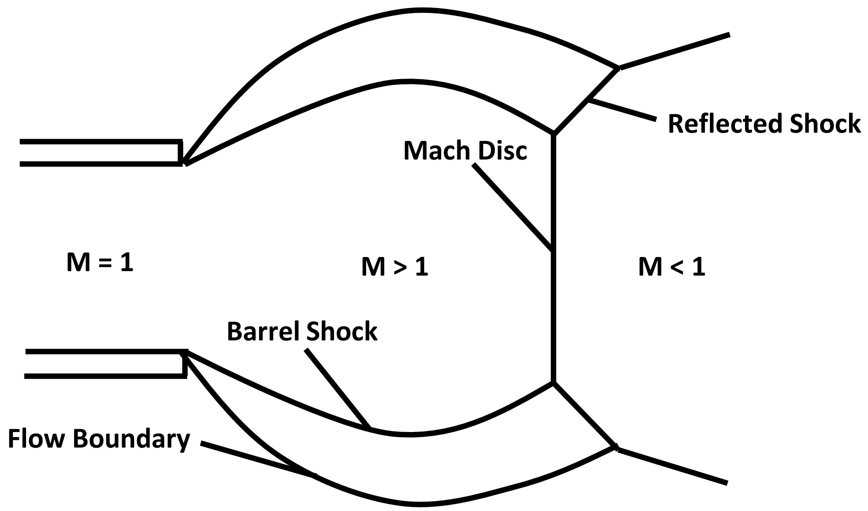
→

$$\frac{P_{nozzle}}{P_{ambient}} > 1.9$$

$\Rightarrow$ underexpanded jet

CFD Modelling Approach – Pseudo Source

- Underexpanded jets occur when the ratio between the nozzle exit and ambient pressures exceeds a critical value, ~1.9 for H_2
- Resulting flow is characterised by a barrel-shaped expansion region close to the nozzle
- Pseudo sources often used to model release downstream of the shock
- One widely used approach is that of Ewan & Moodie (1986)



CFD Modelling Approach – Pseudo Source

- The Ewan & Moodie (1986) pseudo source has the same conditions as the nozzle exit in terms of:
  - mass flow rate
  - velocity
  - temperature
- The release area is then modified to account for jet expansion:

$$A_{source} = A_{nozzle}\left(\frac{P_{nozzle}}{P_{ambient}}\right)$$

- Conditions at the nozzle exit are approximated assuming isentropic expansion from the stagnation conditions

CFD Modelling Approach – Pseudo Source

- The Ewan & Moodie (1986) pseudo source is positioned twice the length of the barrel shock downstream of the nozzle:

$$L = 2 \times \left[0.77d + 0.068d^{1.35}\left(\frac{P_{nozzle}}{P_{ambient}}\right)\right]$$

- Here L is the distance of the pseudo source downstream of the nozzle and d is the nozzle diameter, both in units of mm
- For the Ruggles & Ekoto (2012) jet the pseudo source has/is:
  - 3.4 mm diameter
  - 3.5 mm downstream of nozzle

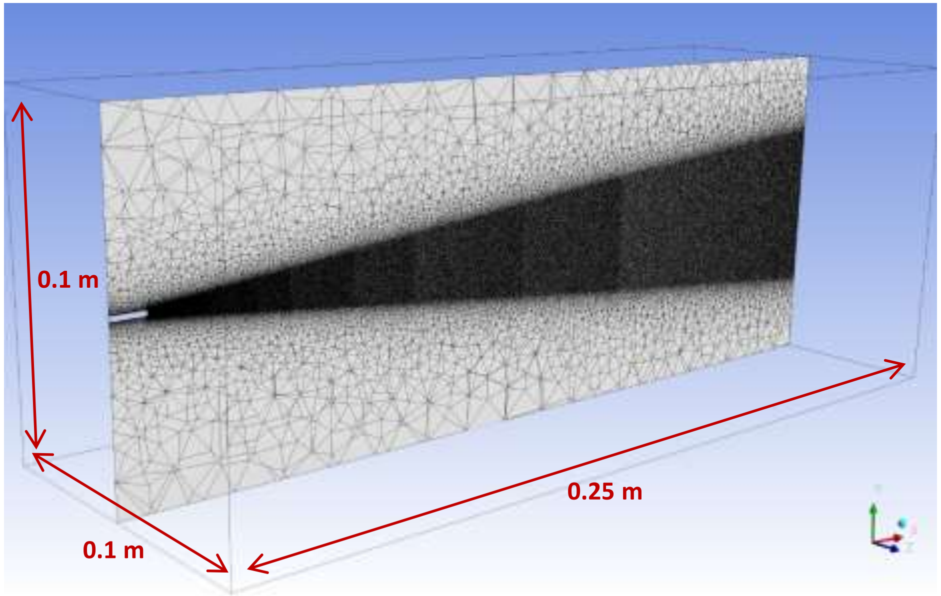
CFD Modelling Approach – Domain

- The jets were simulated in two stages:
  - Stage 1: Nozzle to 0.25 m
  - Stage 2: 0.25 m to 3.5 m
- Allows for greater mesh resolution close to nozzle and barrel-shaped expansion region
- A more coarse mesh can be used further downstream
- Keeps overall mesh size down – adaptive mesh refinement would be an alternative way to achieve this
- Approach is similar to that used by others, e.g. Xu et al. (2005) and Makarov & Molkov (2010)

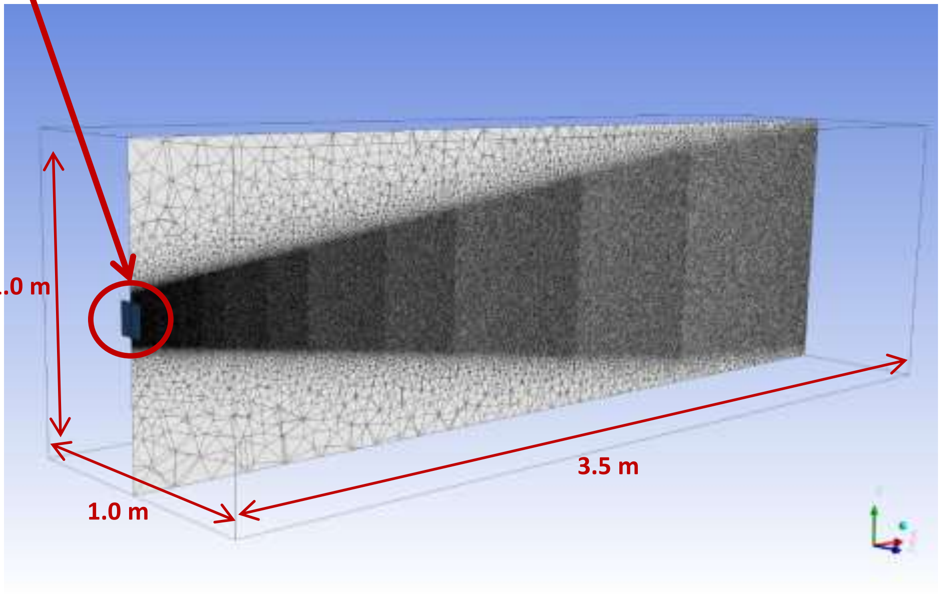
CFD Modelling Approach – Domain

- Conditions at the downstream boundary of Stage 1 are exported and used as an inflow condition for Stage 2 modelling

Near-field jet structure



Far-field H_2 dispersion



CFD Modelling Approach – BC's

- A 0.5 m/s co-flow imposed on the upstream domain boundary
- The domain was also initialised with the same flow condition
- The remaining domain boundaries were assigned as fixed pressure entrainment boundaries at ambient pressure
- The jet inlet was defined with 10% turbulence intensity

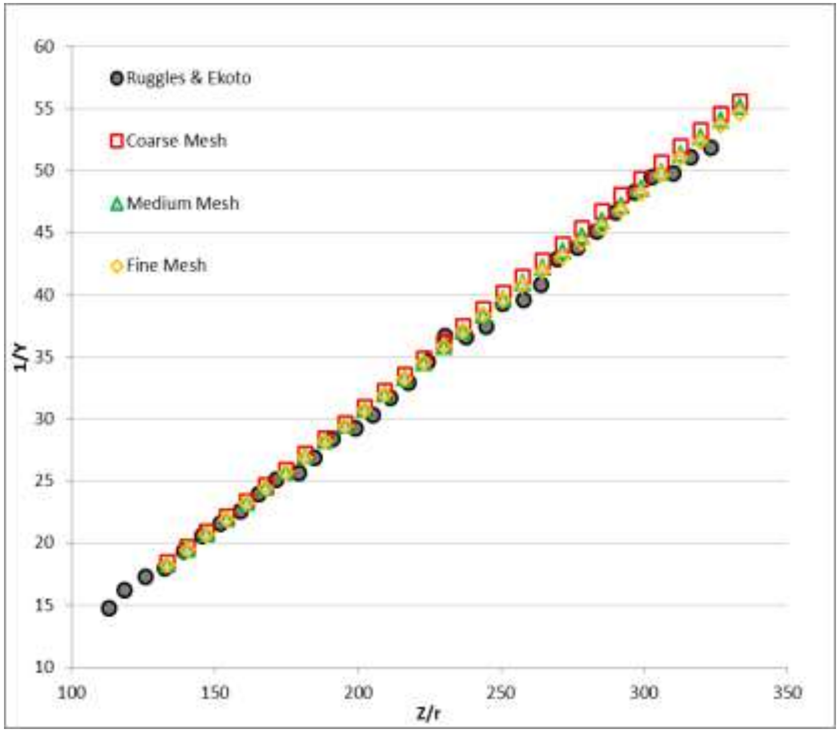
CFD Modelling Approach – Sub-models

- The following sub-models were used in the CFD model set up:
  - Turbulence: standard $k - \varepsilon$ model
  - Heat transfer: ANSYS CFX 16.0 Total Energy model
  - Solver: ANSYS CFX 16.0 High Speed Numerics
  - H_2 distribution: multi-component fluid, scalar transport equation
  - Buoyancy: ANSYS CFX 16.0 full buoyancy model
- Sensitivity analyses were undertaken to assess the impact of:
  - Mesh resolution: near and far field
  - Choice of turbulence model
  - Imposed BCs: co-flow velocity and inlet turbulence intensity

CFD Model Validation & Sensitivity Analyses

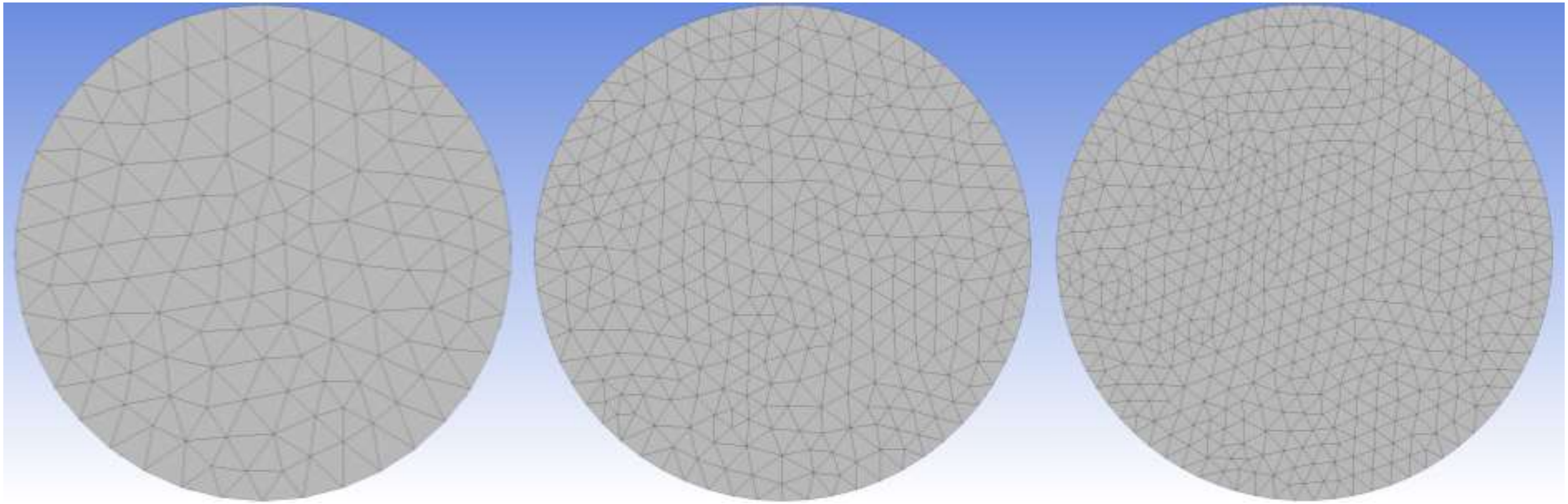
CFD Model Validation

- CFD model of base case validated against Ruggles & Ekoto (2012) data:
  - Near-field H_2 concentration
  - Mach disc size and location
- Three different mesh resolutions also tested in a grid sensitivity study
- Little variation between meshes and good agreement with the measured H_2 concentrations



Sensitivity Analyses – Mesh Resolution

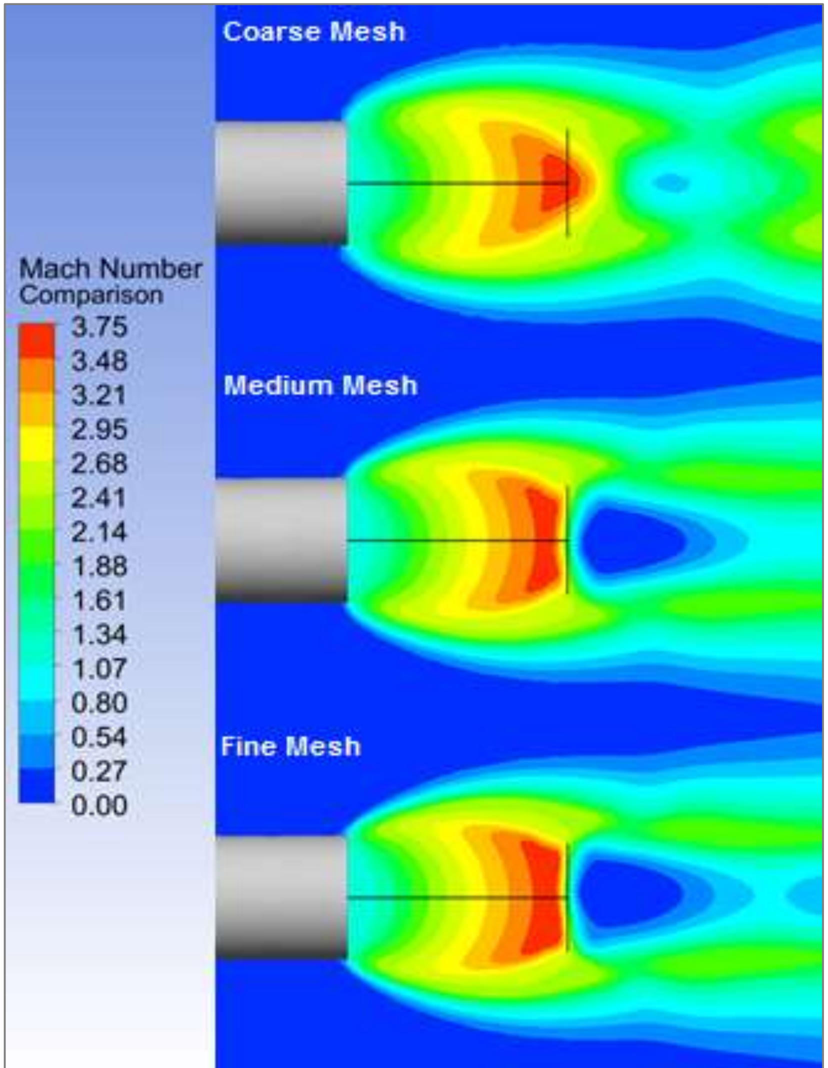
Coarse Medium Fine

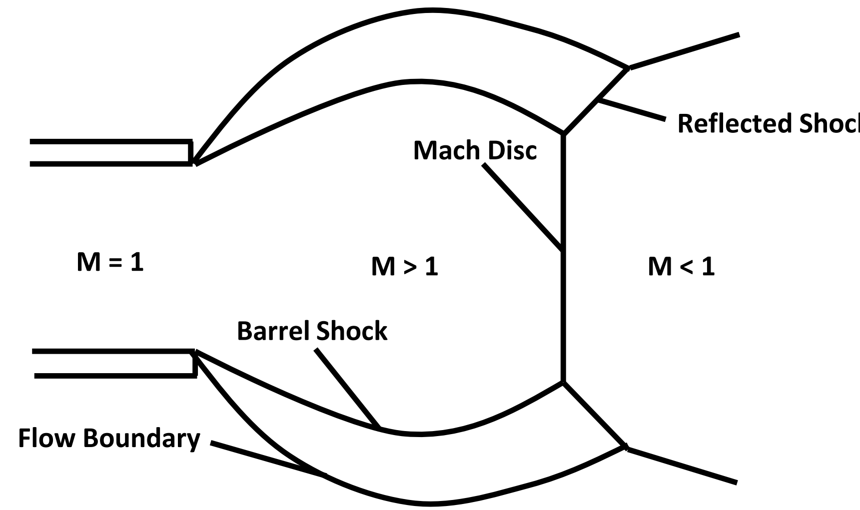


Mesh	Total Node Count	Nodes Resolving Jet Inlet
Coarse	0.3 million	150
Medium	1.0 million	360
Fine	3.8 million	560

- Matrix of 9 simulations with coarse, medium and fine meshes in the near and far field

Sensitivity Analyses – Mesh Resolution





- Measured Mach disc size and location shown by black lines (left)
  - Diameter = 1.3 mm
  - Downstream position = 3.05 mm

Sensitivity Analyses – Mesh Resolution

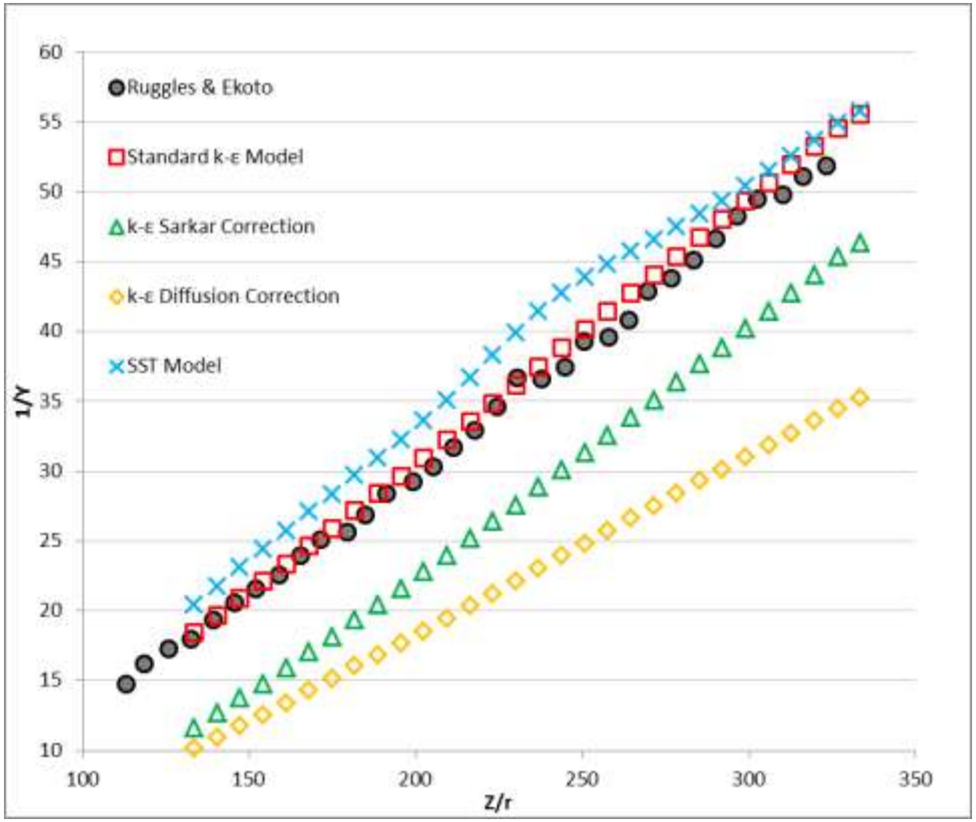
- Mesh sensitivity analysis gave the following ranges of predicted hazard quantities:
  - Flammable volume: 0.141 – 0.156 m^3
  - Hazard distance: 2.73 – 2.75 m
- Largest flammable volume predicted using coarse meshes for both simulation stages
- Impact of mesh resolution on predicted hazard distance is minimal
- Coarse mesh resolutions used for both the near- and far-field simulations with rectangular nozzle releases

Sensitivity Analyses – Turbulence Model

- Sensitivity to the choice of turbulence model also tested
- Four models were assessed:
  - Standard $k - \varepsilon$ model (ANSYS CFX 16.0 formulation)
  - Shear Stress Transport (SST) model (ANSYS CFX 16.0 formulation)
  - Sarkar-corrected $k - \varepsilon$ model (Sarkar et al., 1991)
  - Diffusion-corrected $k - \varepsilon$ model (Pope, 1978; Smith et al., 2004)
- Each model was used to simulate the Ruggles & Ekoto (2012) jet using coarse mesh resolutions

Sensitivity Analyses – Turbulence Model

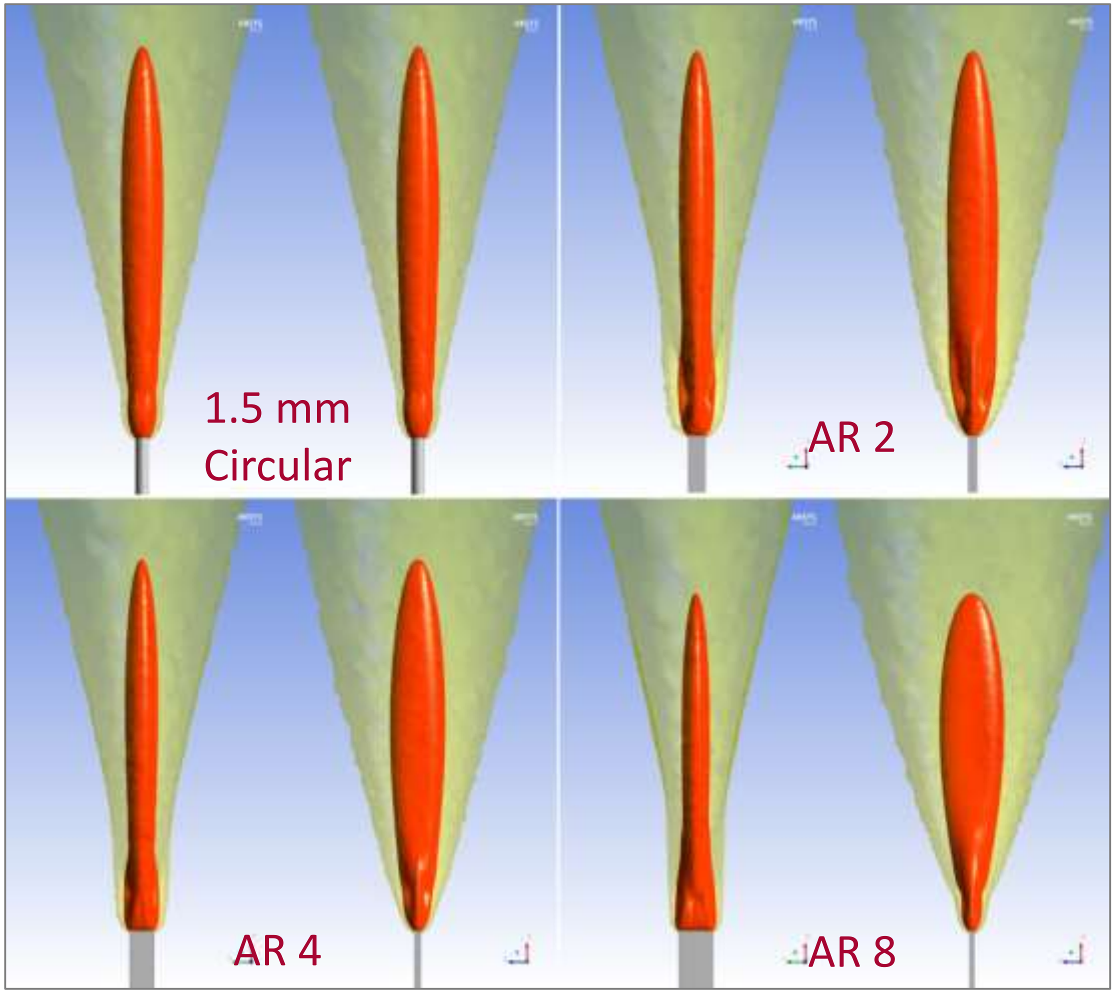
- Results show that the standard $k-\varepsilon$ model results agree most closely with measurements
- SST model slightly under-predicts H_2 concentrations
- The diffusion corrected models over-predict centreline H2 concentration significantly



CFD Modelling Results

Results – Comparison of Nozzle Shapes

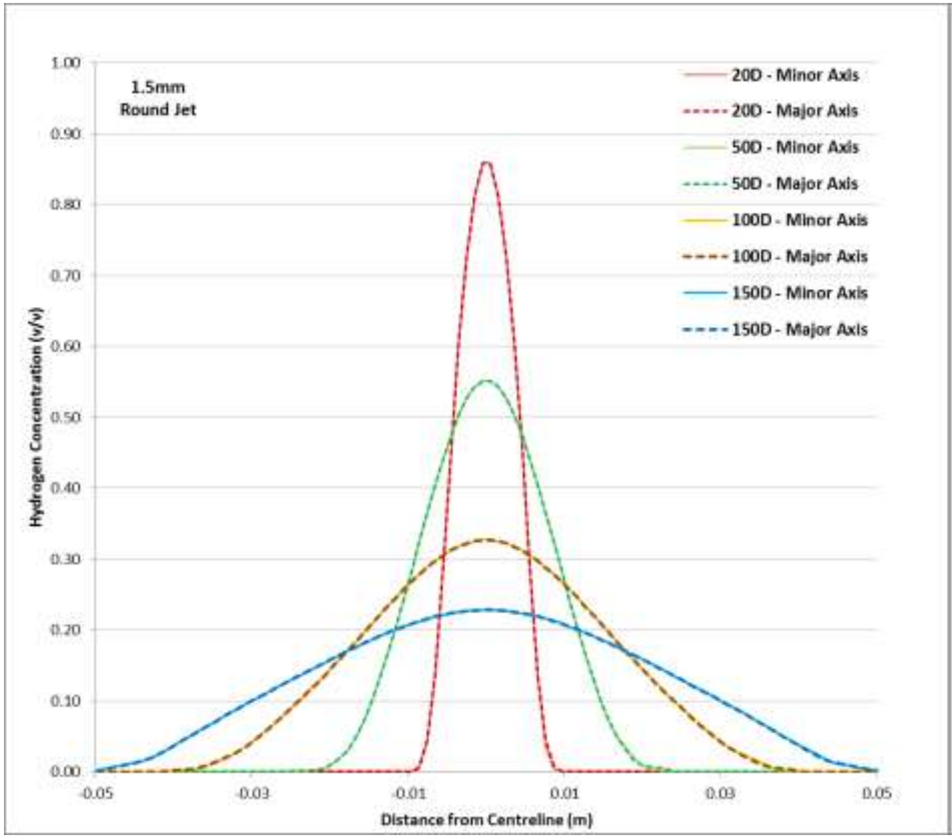
- Nozzle shape has a significant influence on near-field jet structure
- The circular jet is axisymmetric
- The slot jets exhibit an asymmetric shape
- 90˚axis switching: major and minor axes are reversed

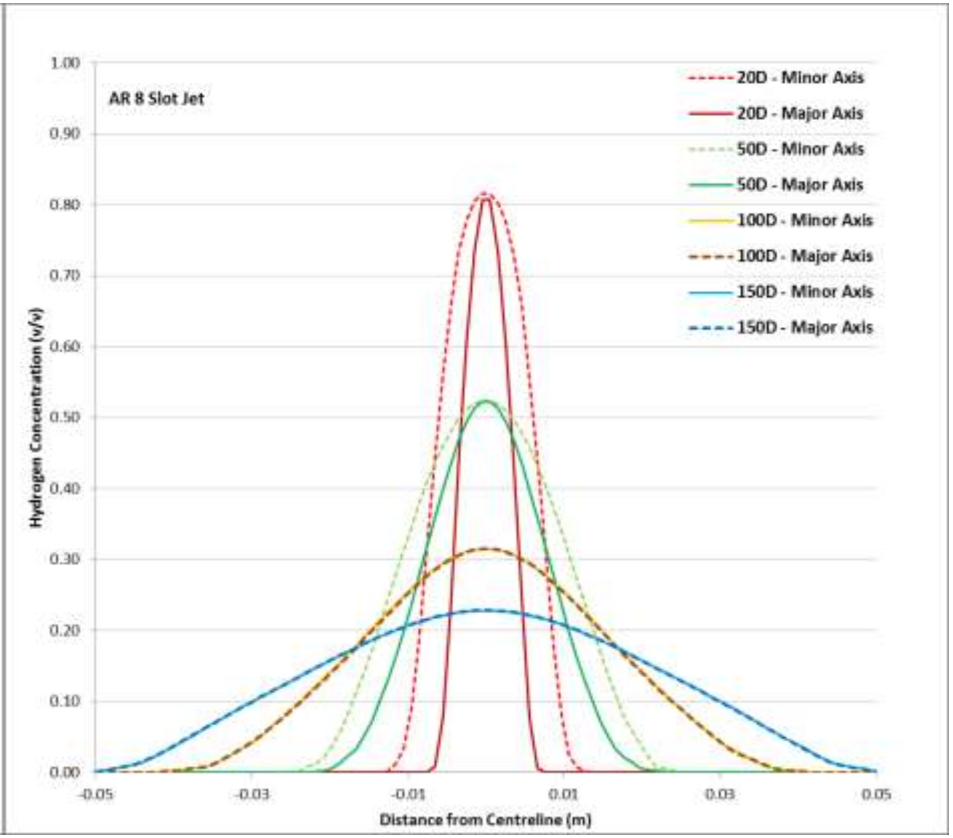


Results – Comparison of Nozzle Shapes

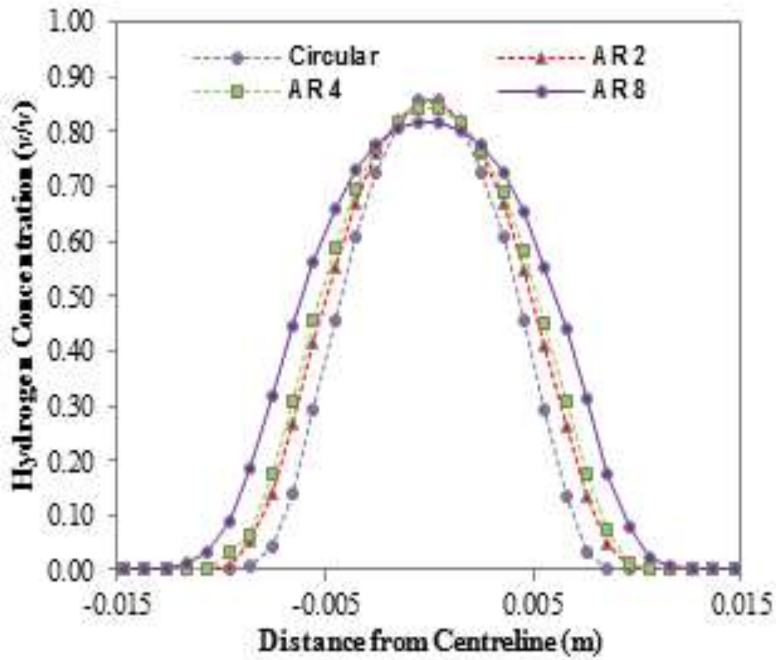
Round jet: 1.5 mm diameter

Slot jet: aspect ratio = 8

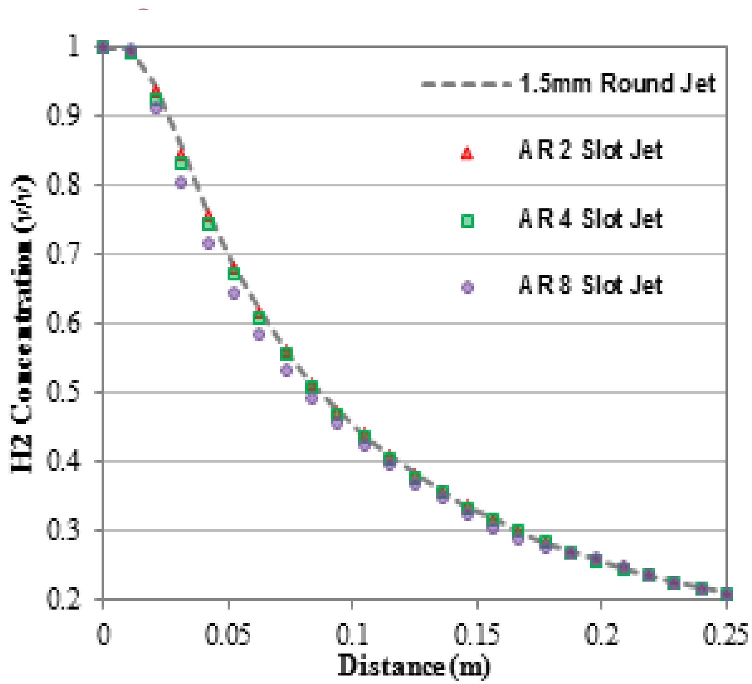




Results – Comparison of Nozzle Shapes



Radial H_2 profile at 0.03 m (Z/r = 20) downstream



Centreline H_2 concentration decay

Results – Hazard Predictions

- The three slot jets and the round jet base case gave very similar hazard quantities
- Using the pseudo source approach gives conservative hazard quantity predictions
- Both Quadvent 2.0 and FreeJet also give conservative results

	1.5mm Round	AR 2 Slot	AR 4 Slot	AR 8 Slot	Pseudo Source	Quadvent 2.0	FreeJet
Hazard Distance (m)	2.73	2.72	2.72	2.72	3.18	2.78	3.36
Hazard Volume (m3)	0.153	0.152	0.150	0.151	0.281	0.277	0.210

Discussion & Conclusions

Conclusions

- Mesh sensitivity analysis shows:
  - A fine mesh is required to capture the barrel shock and Mach disc
  - Resolution of near-nozzle flow has little impact predicted hazard quantities
- Nozzle shape significantly affects near-field dispersion:
  - Jets exiting rectangular openings exhibit 90 ° axis switching
  - Slot jets initial have lower centreline concentration than round jets
  - Releases from rectangular openings are initially asymmetric
- Far-field results are not affected greatly by the nozzle shape
  - Slot jets become axisymmetric around 120 nozzle diameters downstream
  - Predicted distance to ½ LFL and flammable volume were unaffected by the orifice shape

Conclusions

- Ewan & Moodie (1986) pseudo source gives conservative predictions of the flammable volume and distance to ½ LFL
- Compared to the jets modelled directly from the orifice, the pseudo source model gave:
  - ~15% greater distance to ½ LFL
  - ~85% larger flammable volume
- Using a pseudo source can be considered as an appropriate means of modelling underexpanded jet releases from non-circular holes

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