CFD Modelling of Underexpanded Hydrogen Jets Exiting Rectangular Shaped Openings

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Overview
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 H₂ dispersion from underexpanded jets

H₂ 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 $\frac{1}{2}$ LFL < conc$^n$ < UFL)
  – Hazard distance (downstream distance to $\frac{1}{2}$ 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.

<table>
<thead>
<tr>
<th></th>
<th>Ambient</th>
<th>Stagnation</th>
<th>Nozzle Exit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (kPa)</td>
<td>98.37</td>
<td>983.20</td>
<td>515.40</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>296.0</td>
<td>295.4</td>
<td>244.8</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>N/A</td>
<td>N/A</td>
<td>1202.7</td>
</tr>
</tbody>
</table>

\[
\frac{P_{\text{nozzle}}}{P_{\text{ambient}}} > 1.9
\]

⇒ underexpanded jet

Ruggles & Ekoto (2012) Data
• Underexpanded jets occur when the ratio between the nozzle exit and ambient pressures exceeds a critical value, ~1.9 for $\text{H}_2$
• 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)
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.
The Ewan & Moodie (1986) pseudo source is positioned twice the length of the barrel shock downstream of the nozzle:

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

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
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 $\text{H}_2$ 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
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\textsubscript{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\textsubscript{2} concentrations
Sensitivity Analyses – Mesh Resolution

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

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Total Node Count</th>
<th>Nodes Resolving Jet Inlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>0.3 million</td>
<td>150</td>
</tr>
<tr>
<td>Medium</td>
<td>1.0 million</td>
<td>360</td>
</tr>
<tr>
<td>Fine</td>
<td>3.8 million</td>
<td>560</td>
</tr>
</tbody>
</table>
Sensitivity Analyses – Mesh Resolution

- Measured Mach disc size and location shown by black lines (left)
  - Diameter = 1.3 mm
  - Downstream position = 3.05 mm
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 $H_2$ 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 $\text{H}_2$ profile at 0.03 m $(Z/r = 20)$ downstream

Centreline $\text{H}_2$ 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.

<table>
<thead>
<tr>
<th>Hazard Distance (m)</th>
<th>1.5mm Round</th>
<th>AR 2 Slot</th>
<th>AR 4 Slot</th>
<th>AR 8 Slot</th>
<th>Pseudo Source</th>
<th>Quadvent 2.0</th>
<th>FreeJet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hazard Volume (m³)</td>
<td>2.73</td>
<td>2.72</td>
<td>2.72</td>
<td>2.72</td>
<td>3.18</td>
<td>2.78</td>
<td>3.36</td>
</tr>
<tr>
<td></td>
<td>0.153</td>
<td>0.152</td>
<td>0.150</td>
<td>0.151</td>
<td>0.281</td>
<td>0.277</td>
<td>0.210</td>
</tr>
</tbody>
</table>
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 \( \frac{1}{2} \) LFL

• Compared to the jets modelled directly from the orifice, the pseudo source model gave:
  – ~15% greater distance to \( \frac{1}{2} \) 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
References


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