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Notional Nozzle Models for Hydrogen Releases from High Pressure Systems

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Evaluation of notional nozzle approaches for CFD simulations of free-shear under-expanded hydrogen jets

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Notional Nozzle Concept

Need for reasonable computer run-times, for engineering applications

Replacement of the actual release nozzle by a notional one

The notional nozzle does not exist in real jets since it is based on strong simplifications/assumptions:

- uniform velocity profile
- uniform concentration profile
- flow properties from conservation equations applied on the jet centreline

Under-expanded jet release
Level 1: “reservoir” conditions
Level 2: real orifice
Level 3: notional nozzle location
5 Notional Nozzle Models

- **Birch et al. (1984):** Conservation of mass, temperature at notional nozzle equal to atmospheric
- **Birch et al. (1987):** Conservation of mass, conservation of momentum, temperature at notional nozzle equal to atmospheric
- **Ewan and Moodie (1986):** Conservation of mass, temperature at notional nozzle equal to the one at the actual release nozzle
- **Schefer et al. (2007):** Conservation of mass, conservation of momentum, real gas (Abel-Noble equation of state), temperature at notional nozzle equal to atmospheric
- **Harstad and Bellan (2006):** Conservation of mass, conservation of momentum, conservation of energy, location just after the Mach disk (Low flow speed).
3 Turbulence Models

- Standard $k-\varepsilon$
- Shear Stress Transport (SST)
- Baseline (BSL) $k-\omega$ model

RNG model was abandoned because grid independence could not be reached

<table>
<thead>
<tr>
<th></th>
<th>Coarse</th>
<th>Fine</th>
<th>Finer</th>
<th>Finest</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total number of nodes</td>
<td>47.500</td>
<td>68.800</td>
<td>179.300</td>
<td>533.300</td>
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<td>Number of nodes in the</td>
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<td>72.100</td>
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<td>conical geometry</td>
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<td>Minimum (10^{-4} m) and</td>
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<td>maximum (10^{-1} m) grid</td>
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<td>geometry</td>
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</table>
## FZK/KIT Experiments

<table>
<thead>
<tr>
<th>Test No.</th>
<th>Nozzle Diameter (mm)</th>
<th>Pressure (bar)</th>
<th>Flow rate (10^-3 kg/s)</th>
<th>Distance from nozzle (m)</th>
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</thead>
<tbody>
<tr>
<td>HD35-37</td>
<td>1</td>
<td>54.6</td>
<td>2.46</td>
<td>0.75</td>
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<td></td>
<td></td>
<td>52.1</td>
<td>2.35</td>
<td>1.5</td>
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<tr>
<td></td>
<td></td>
<td>53.1</td>
<td>2.39</td>
<td>2.25</td>
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<tr>
<td>HD00-02</td>
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<td>1.5</td>
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<td></td>
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<td>99.6</td>
<td>2.53</td>
<td>2.25</td>
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<tr>
<td>HD22-24</td>
<td>0.25</td>
<td>162.8</td>
<td>0.46</td>
<td>0.75</td>
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<td></td>
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<td>160.4</td>
<td>0.45</td>
<td>1.5</td>
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<tr>
<td></td>
<td></td>
<td>162.1</td>
<td>0.46</td>
<td>2.25</td>
</tr>
</tbody>
</table>

### Experimental conditions

- **Simulation Pressure (bar):**
  - 53.27
  - 113.3
  - 102.2
  - 162.0
## Conditions at the Notional Nozzle

<table>
<thead>
<tr>
<th>Approach</th>
<th>Temperature (K)</th>
<th>Density (kg/m$^3$)</th>
<th>Velocity (m/s)</th>
<th>Diameter (10$^{-3}$ m)</th>
<th>Mass flow rate (10$^{-3}$ kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>HD35-37 (1 mm nozzle diameter, 53.27 bar)</strong></td>
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<tr>
<td>Birch1984</td>
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<td>2.4</td>
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<td><strong>HD22-24 (0.25 mm nozzle diameter, 162 bar)</strong></td>
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<td></td>
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</tr>
<tr>
<td>Birch1984</td>
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<td>Schefer</td>
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<td>0.0854</td>
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<td>1.827</td>
<td>0.46</td>
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<td>Harstad</td>
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<td>3.645</td>
<td>0.46</td>
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<td>Exp. data</td>
<td>234</td>
<td>7.76</td>
<td>1239</td>
<td>0.25</td>
<td>0.46</td>
</tr>
</tbody>
</table>
**Experiment/Simulation comparison with statistical analysis**

\[
MG = \exp\left(\ln V_o - \ln V_p\right) \quad VG = \exp\left[\left(\ln V_o - \ln V_p\right)^2\right]
\]

- Geometric Mean Bias (MG): it measures relative mean bias and indicates only systematic errors based on a logarithmic scale.

- Geometric Mean Variance (VG): it measures relative scatter.

- Vo is the observed (experimental) value and Vp is the predicted (numerical) value.
HD35-37: 1 mm nozzle; 53 bar

Green → SST
Blue → BSL
Red → k-ε

MG<1 over-prediction
MG>1 under-prediction
HD35-37: 1 mm nozzle; 53 bar

[Graph showing geometric mean variance (VG) vs. geometric mean bias (MG) for HD35-37 with data points for Birch 1987, Birch 1984, Ewan, Schefer, Harstad, and Parabola.]

Green → SST
Blue → BSL
Red → k-ε

MG<1 over-prediction
MG>1 under-prediction
HD35-37: 1 mm nozzle; 53 bar

Spreading rates: the value of the radial distance from the centreline where H2 mass fraction and velocity are half their centreline value. (Green $\rightarrow$ SST Blue $\rightarrow$ BSL Red $\rightarrow$ k-\(\varepsilon\))
HD00-02: 0.75 mm nozzle, ~100-112 bar

**Diagram: Geometric Mean Variance (VG) vs. Geometric Mean Bias (MG)**

- **Green → SST**
- **Blue → BSL**
- **Red → k-ε**
HD00-02: 0.75 mm nozzle, ~100-112 bar

HD00-02: Centreline H₂ mass fraction

- Birch 1987
- Birch 1984
- Ewan
- Schefer
- Harstad
- Parabola

Geometric Mean Variance (VG) vs. Geometric Mean Bias (MG)

Green → SST
Blue → BSL
Red → k-ε
HD00-02: 0.75 mm nozzle, ~100-112 bar

Spreading rates: the value of the radial distance from the centreline where H2 mass fraction and velocity are half their centreline value.

(Green → SST Blue → BSL Red → k-ε)
HD22-24: 0.25 mm nozzle, ~161 bar

HD22-24: Centreline flow velocity

- Birch 1987
- Birch 1984
- Ewan
- Schefer
- Harstad
- Parabola

Green $\rightarrow$ SST
Blue $\rightarrow$ BSL
Red $\rightarrow$ k-\(\varepsilon\)
In general simulation results are less accurate than at lower pressure and with larger diameter.

By comparison of Schefer and Birch87: need for real gas equation at high pressure
Identified trends

For higher pressure and smaller diameter, the accuracy decreases.

Accuracy of the notional nozzle models in the following order, given the same turbulence model: Birch87/Schefer, Birch84/Ewan, Harstad.

Accuracy of turbulence models. For the concentration, SST and BSL perform in general better than \( k-\varepsilon \). For the flow velocity, the results give less uniform indications. In some cases, \( k-\varepsilon \) is the most accurate model.

Those conclusions are valid for the 3 cases that have been considered in the investigation and for the selected approach (e.g. unstructured mesh). Other cases should be considered to give more general validity to the conclusions e.g. very high pressure (500-700 bar), different diameter size, jet impingement with obstacles/walls.
GAPS

Validation of more recent notional nozzle models e.g. Molkov’s

Validation with comparison for other extremely relevant parameter for the combustion e.g. not only concentration and flow speed but also turbulence.

Validation with broader range of conditions: very high pressure (500-700 bar), different diameter size, jet impingement with obstacles/walls.

Definition of criteria to help to identify the best modelling strategy for each application: which notional nozzle? notional nozzle or real nozzle?