Modelling Vented Hydrogen Deflagrations:

The influence of user variability and model sensitivity

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• Introduction to HySEA
• Summary of the HySEA modelling exercises
  – Homogeneous mixtures
  – Inhomogeneous gas clouds
• CFD Modelling performed by HSE
  – Key modelling decisions and their influence
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• Blind-prediction exercise results
• Summary & Discussion
Overview

- Presentation focusses on HySEA project
- Emphasis on modelling performed as part of the HySEA blind-prediction modelling exercises
- Highlights a number of modelling decisions which can have a significant impact on model results
- Presents model sensitivity analyses for the HySEA blind-prediction studies
- Assesses the user-variability in model predictions submitted to the HySEA first modelling exercise
HySEA

- **Hydrogen Safety for Energy Applications (HySEA)**
- Aimed at studying vented deflagrations in containers and enclosures for hydrogen energy applications
- Unobstructed and obstructed tests to assess the effects of obstacles representative of industrial systems
- Development and validation of predictive models through comparison to existing data and experimental results generated through HySEA test programs
- Modelling blind-prediction studies for inter-model, and inter-user comparison
Two blind-prediction studies conducted to date
- Homogeneous H₂/air mixture (BE1)
- Inhomogeneous H₂/air cloud (BE2)

Model predictions submitted for the 1st exercise by a range of academic, commercial and regulatory groups

Results of the 1st exercise and the corresponding experimental tests have been presented at UKELG and ICHS 2017

Analysis and publication of the results from the 2nd exercise is in ongoing
BE1 – Homogeneous Mixtures

- Blind-prediction of vented hydrogen deflagrations in a 20 ft. ISO container
  - One unobstructed scenario
  - One obstructed case with a cylinder bundle inside the container
- Homogeneously mixed, quiescent hydrogen/air mixture at a concentration of 15±0.2% v/v
- Ignition at the centre of the container back wall
- Venting through open container doors

Figure taken from HySEA 1st blind-prediction exercise instructions [1]
BE2 – Inhomogeneous Clouds

• Blind-prediction of vented hydrogen deflagrations in a 20 ft. ISO container
  – One unobstructed scenario
  – One obstructed scenario with a pipe rack inside the container

• Vertically-oriented jet release of hydrogen to form stratified, inhomogeneous gas cloud
  – 450 s release duration
  – 1.33 g/s release rate
  – Nominal hydrogen concentration at time of ignition expected to be ~21% v/v

• Upper back wall ignition 30 s after the end of the hydrogen release

• Explosion venting through six 1 m² pressure relief panels fitted into the top of the container
Modelling by HSE

• FLACS simulations performed and results submitted for both blind-prediction exercises
  – k-ε turbulence model
  – Default time-stepping settings
  – Euler boundary conditions
  – Initial turbulence length scale set to 10% of the grid cell size

• Model sensitivity to grid resolution tested for obstructed and unobstructed cases in both exercises

• Influence of geometry representation and FLACS porosity model assessed

• Sensitivity to domain size and the type of boundary condition applied in the simulations also investigated
Modelling by HSE – BE1

- Geometry replicated as closely as possible in the model
- Limited by the available geometry-creation tools in FLACS, so corrugated walls represented crudely
Modelling by HSE – BE1

- 20 cm
- 10 cm
- 5 cm
- 2.5 cm
• Very different turbulence generation depending on mesh resolution
• Has significant impact on resulting overpressure predictions
Modelling by HSE – BE1 Unobstructed

20 cm mesh

5 cm mesh
Modelling by HSE – BE1 Unobstructed

- Simulations show clear grid dependence
- Pressure traces different across all meshes
- Max. pressure in the container shows no trend with grid refinement
- Approx. factor of 2 difference in peak overpressure across mesh resolutions tested

<table>
<thead>
<tr>
<th>Mesh Size (cm)</th>
<th>20</th>
<th>10</th>
<th>5</th>
<th>2.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Pressure (barg)</td>
<td>0.027</td>
<td>0.016</td>
<td>0.043</td>
<td>0.057</td>
</tr>
</tbody>
</table>
Grid choice has a significant impact on geometry resolution.

FLACS porosity model intended to handle this by introduction of sub-grid-scale effects.

However, results show very different turbulence generation and explosion overpressures for the different meshes.
• Significant differences in turbulence generation at container walls (as before) and around bottle bundle obstruction
Modelling by HSE – BE1 Obstructed

- Higher turbulence velocities predicted around the cylinder bundle obstacle for the finer mesh
Simulations show grid dependence

Pressure traces different across all meshes

Max. pressure in the container very similar for all but the 10 cm mesh

Whilst the peak pressure is predicted to be similar across most meshes, the pressure traces are so different that this appears coincidental

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<tbody>
<tr>
<td>Max. Pressure (barg)</td>
<td>0.101</td>
<td>0.036</td>
<td>0.106</td>
<td>0.092</td>
</tr>
</tbody>
</table>
Modelling by HSE – BE2

- Geometry for 2\textsuperscript{nd} exercise is a slightly modified version of that used for the 1\textsuperscript{st} blind-prediction study
- Again, geometry details are defined in the model in as much detail as possible
- Simulations performed as a dispersion calculation followed by a separate explosion calculation
- Different meshes used for the two stages of simulation with interpolation of the dispersion results on to the explosion calculation mesh
Modelling by HSE – BE2

- Additional features of geometry for the 2\textsuperscript{nd} exercise include:
  - Closed container doors
  - Explosion vent panel openings in container ceiling
  - Holes along side of container to allow air to escape during H\textsubscript{2} jet release

- Corrugated walls remain crudely represented as was the case for the 1\textsuperscript{st} blind prediction

- Differences in resolution of small geometrical features with different meshes remains, as does reliance on the FLACS porosity sub-model
Modelling by HSE – BE2 Unobstructed

- **t = 10 s**
  - ![Diagram at t = 10 s](image1)

- **t = 180 s**
  - ![Diagram at t = 180 s](image2)

- **t = 450 s (end of H₂ release)**
  - ![Diagram at t = 450 s](image3)

- **t = 480 s (time of ignition)**
  - ![Diagram at t = 480 s](image4)
Interpolated concentrations differ significantly across meshes.

Only the 10 cm mesh gives initial $\text{H}_2$ concentrations for the explosion simulation that are close to those at the end of the dispersion calculation.

This has a large influence on the resulting overpressures.
Modelling by HSE – BE2 Unobstructed

- Pressure traces for sensors nearest ignition location show different behaviour for different meshes.
- Given the differences in the initial $H_2$ concentrations, this is not a surprising result.
- Max. overpressure at these sensors ranges by approx. a factor of 4 for the different mesh resolutions used.

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<th>20</th>
<th>15</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Pressure (barg)</td>
<td>1.966</td>
<td>0.598</td>
<td>2.115</td>
<td>0.526</td>
</tr>
</tbody>
</table>
• Largest overpressures predicted at sensors furthest from ignition location (near opposite end of the ISO container)
• Again there are significant differences between the pressure traces predicted for different meshes
• Large variation in max. overpressure across mesh resolutions, with no trend observed

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<th>15</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. Pressure (barg)</td>
<td>4.201</td>
<td>1.591</td>
<td>8.266</td>
<td>0.798</td>
</tr>
</tbody>
</table>
Modelling by HSE – BE2 Obstructed

- Similar behaviour to unobstructed test regarding interpolation of dispersion results onto explosion meshes
- Only the 10 cm mesh gives initial H$_2$ concentrations for the explosion calculation that are similar to those at the end of the dispersion simulation
- The qualitative behaviour of the H$_2$ stratification is not correctly captured, with the exception of the 10 cm mesh case
Modelling by HSE – BE2 Obstructed

- General shape of pressure trace curves could be regarded as reasonably similar
- Differences in predicted max. overpressure significant for different meshes
- No convergence towards a solution as mesh is refined
- Illustrates large mesh sensitivity on predicted overpressure
Blind-prediction Results – BE1

- Significant differences between model predictions, approx. factor of 40 across all models/users
- All modellers predicted the correct trend moving from unobstructed to obstructed, i.e. an increase in peak overpressure
- M-01, M-02, M-04, M-05 and M-10 all used FLACS (various versions)
- Demonstrates effects of user variability

Figure taken from Skjold et al. (2017) [2]
Summary & Discussion

• It has been demonstrated that significant mesh sensitivity exists in the modelling of the HySEA exercises performed by HSE

• FLACS grid sensitivity demonstrated by two other modelling groups who submitted results to the 1st blind-prediction

• A third modelling group, also using FLACS, reported grid independent results for the 1st blind-prediction study

• Blind-prediction results show large variation in predicted max. overpressures
  – Approx. factor of 40 difference

• HySEA modelling exercise shows that different users can produce very different results, even when using the same model
Summary & Discussion

• Why do such large differences exist between results generated by users of the same model?
  – Different decisions about the importance of geometry elements
  – Different interpretations of model user guidelines
  – Different choices of computational mesh
  – Different settings for initial conditions

• How can consistency in modelling by users of the same model be improved?
  – Improved user guidelines
  – More extensive dissemination of model validation
  – Published model validation and sensitivity analyses

• If there are such extensive sensitivities within models and dependencies on the model user, how can we rely on model predictions in practice, e.g. for an offshore explosion QRA?
References


Questions?