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HSE

Modelling Vented Hydrogen Deflagrations:

The influence of user variability and model sensitivity

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  - Homogeneous mixtures
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- Summary & Discussion

Overview

HSE

- 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

HSE

- ***Hy**drogen **S**afety for **E**nergy **A**pplications* (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

HySEA Modelling Exercises

- Two blind-prediction studies conducted to date
  - Homogeneous H_2/air mixture (BE1)
  - Inhomogeneous H_2/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

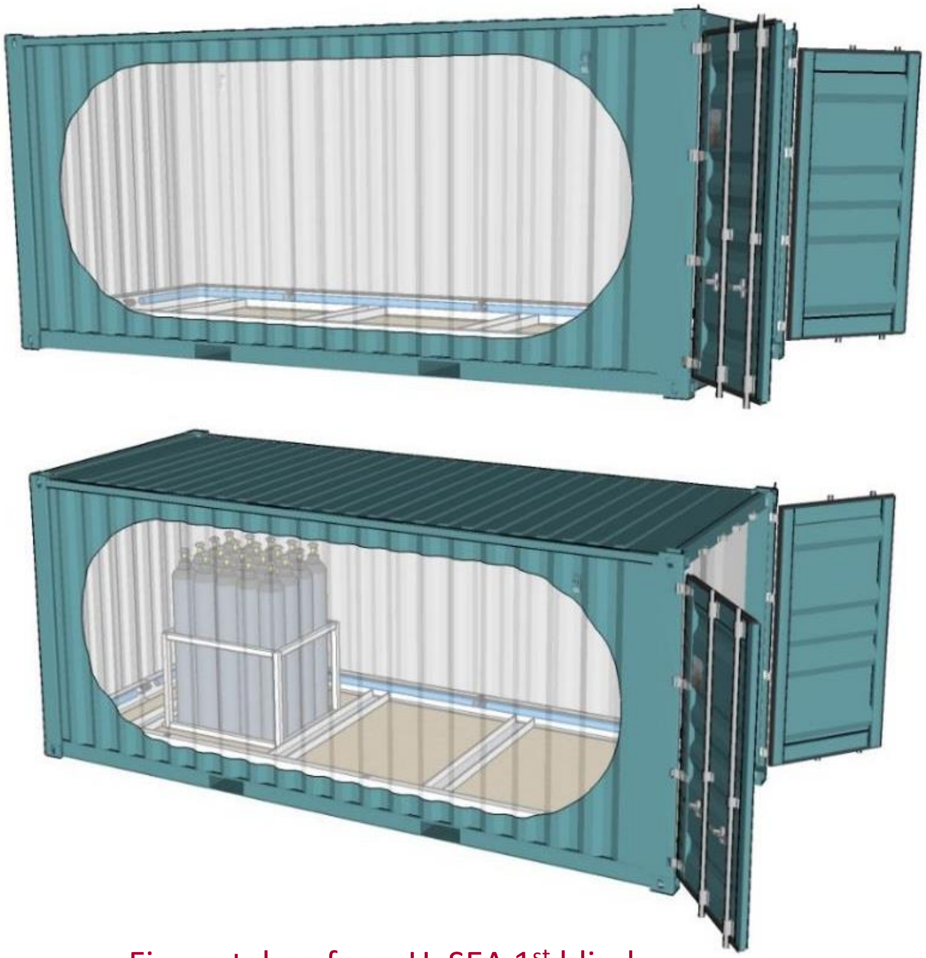


Figure taken from HySEA 1st blind-prediction exercise instructions [1]

- 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

BE2 – Inhomogeneous Clouds

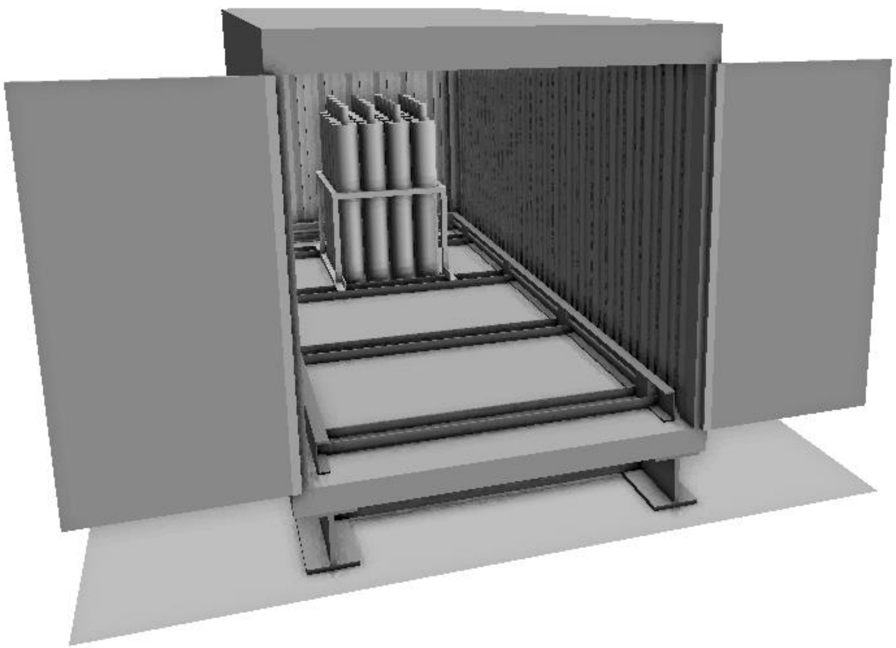
- Blind-prediction of vented hydrogen deflagrations in a 20 ft. ISO container
  - One unobstructed scenario
  - One obstructed scenario with a pipe rack inside the container
- Vertically-oriented jet release of hydrogen to form stratified, inhomogeneous gas cloud
  - 450 s release duration
  - 1.33 g/s 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 m^2 pressure relief panels fitted into the top of the container

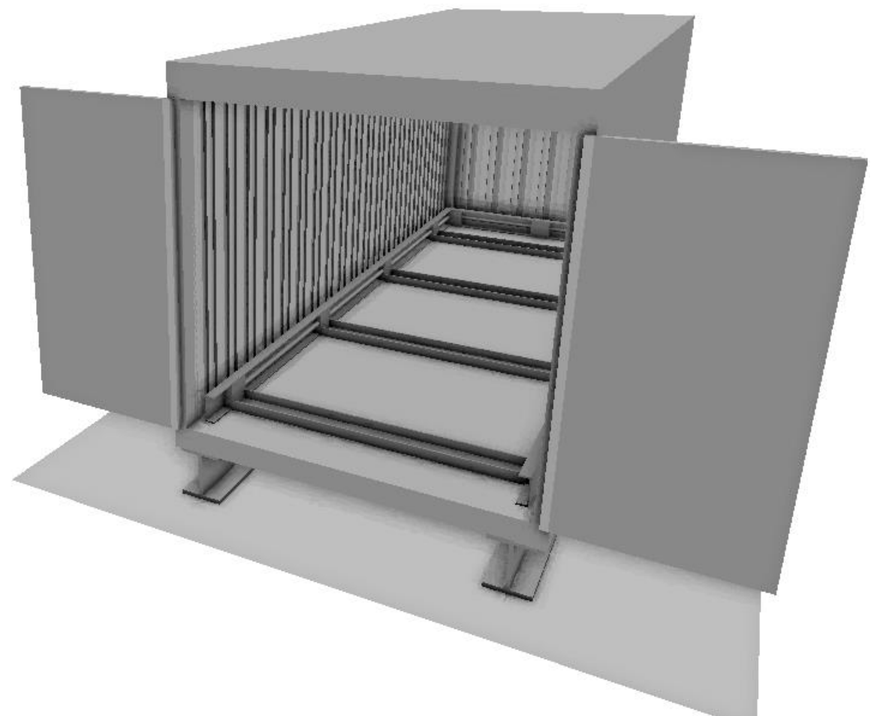
Modelling by HSE

- 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

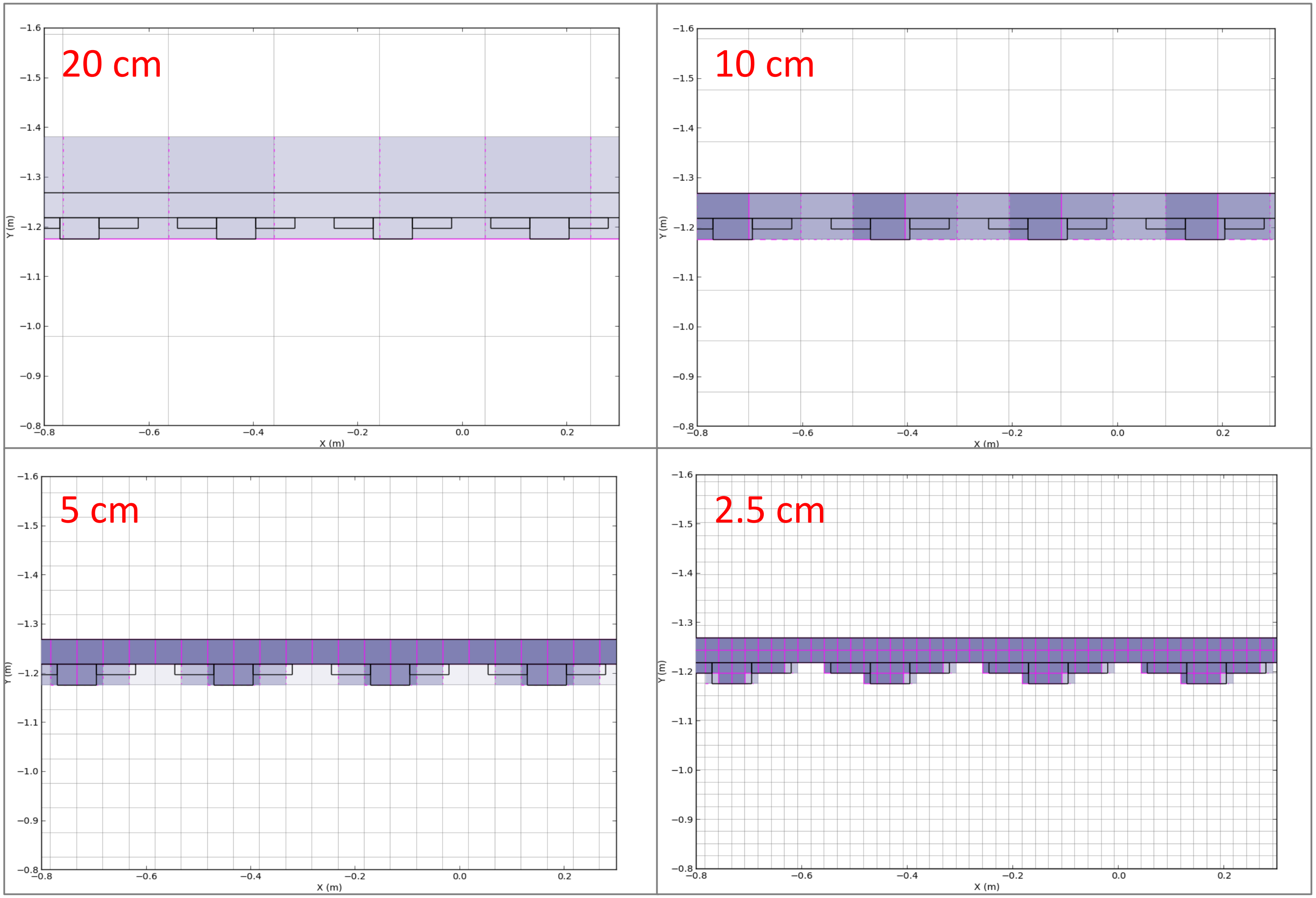
Modelling by HSE – BE1

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



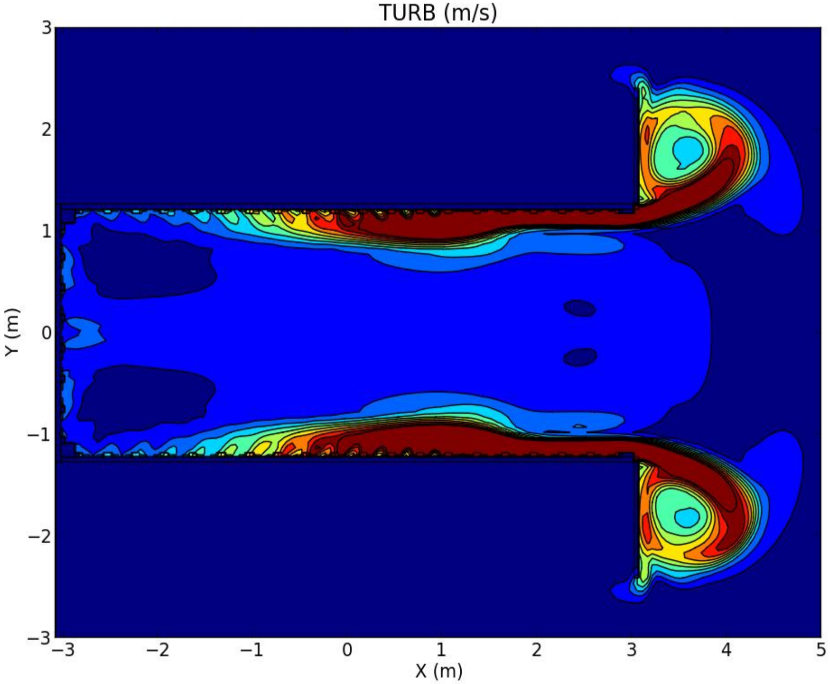


Modelling by HSE – BE1

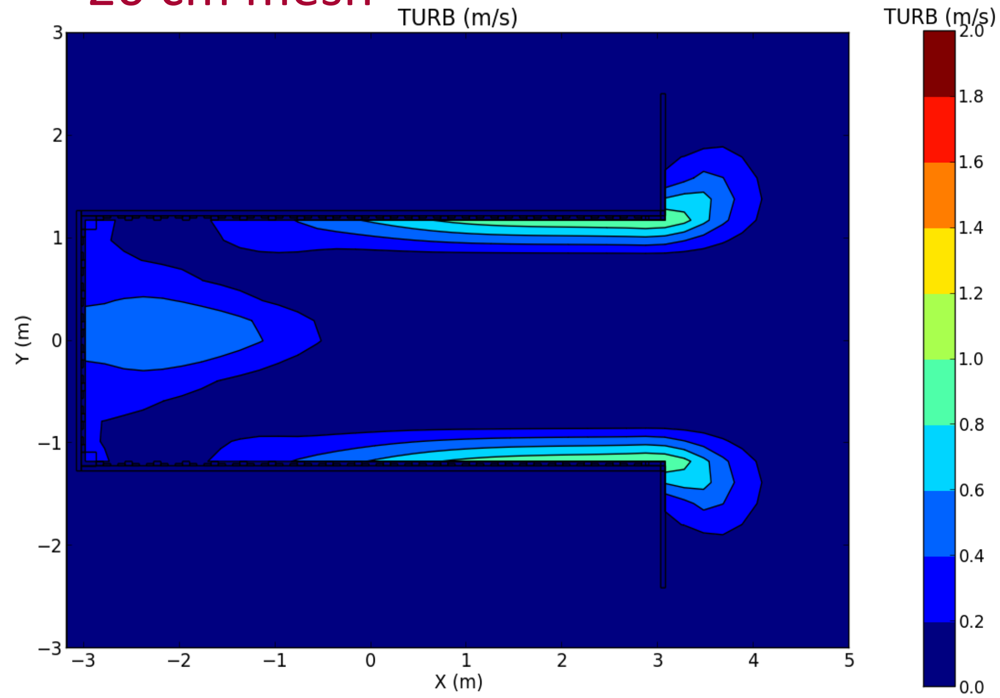


Modelling by HSE – BE1 Unobstructed

5 cm mesh



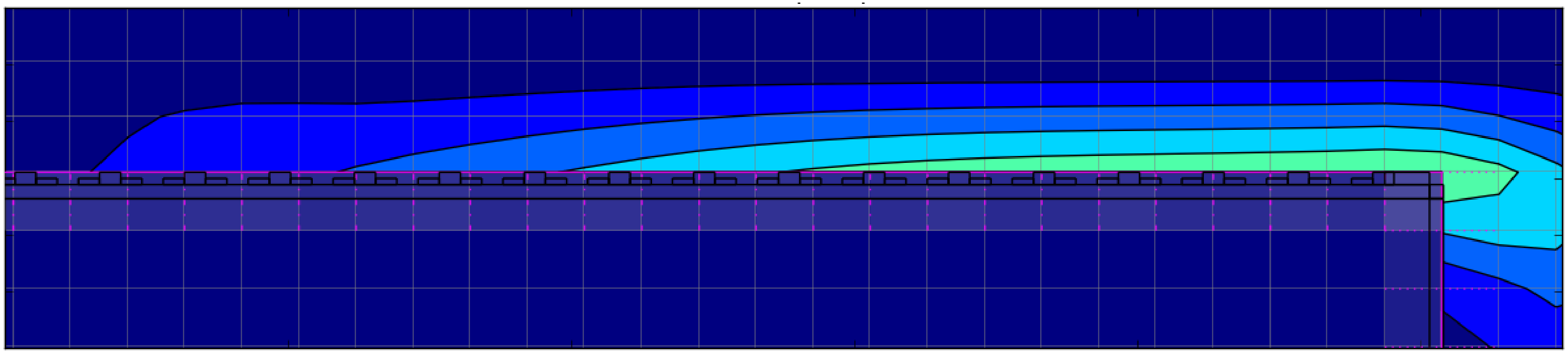
20 cm mesh



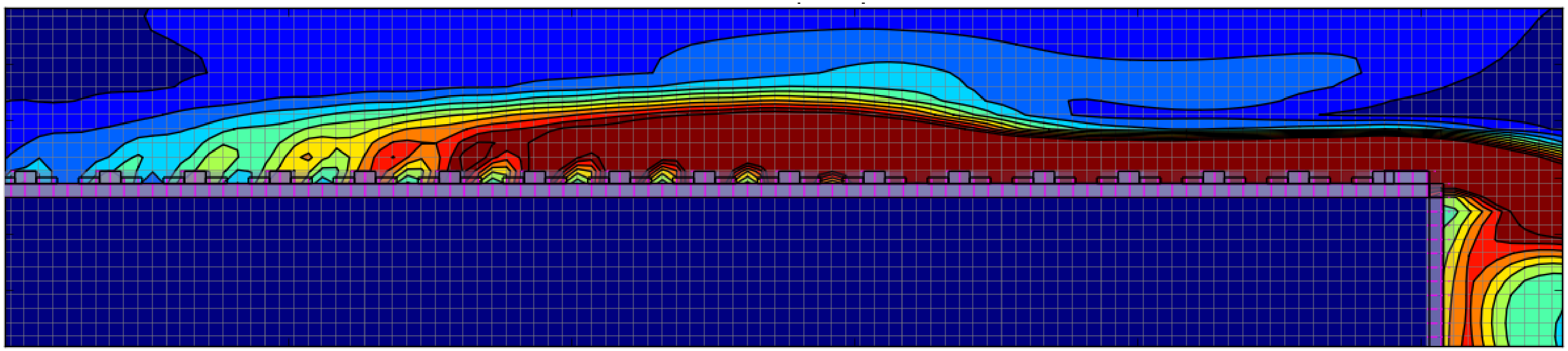
- Very different turbulence generation depending on mesh resolution
- Has significant impact on resulting overpressure predictions

Modelling by HSE – BE1 Unobstructed

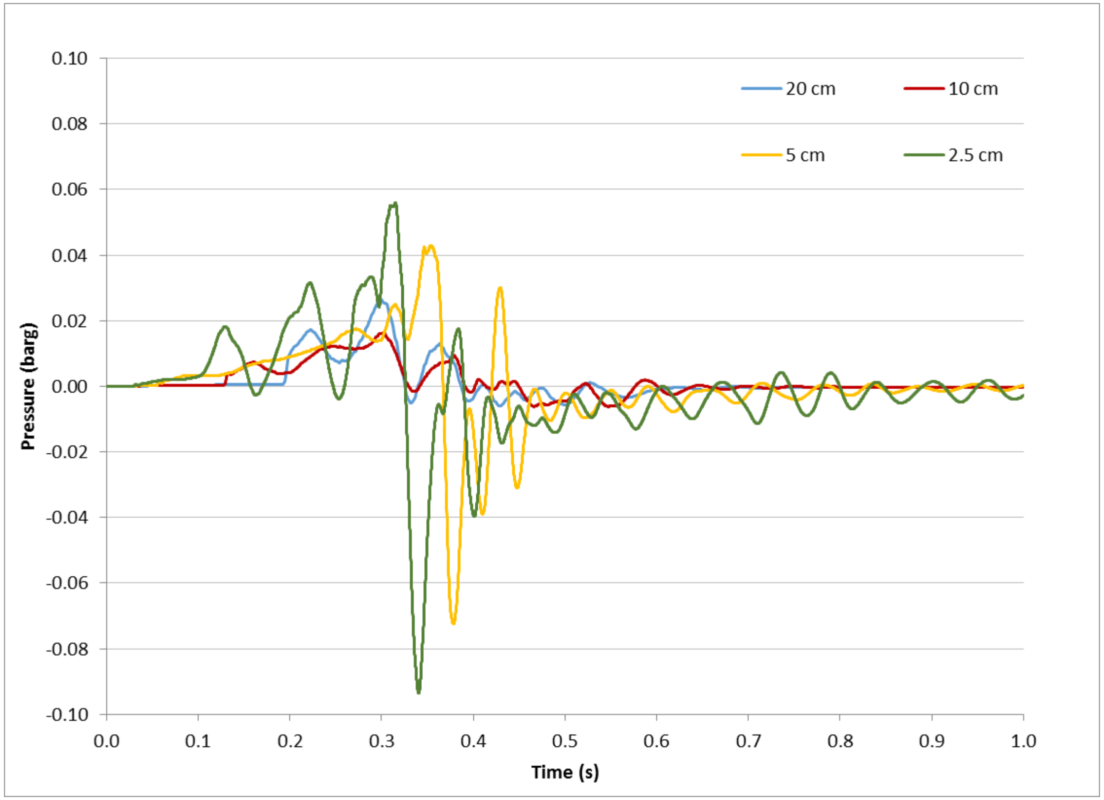
20 cm mesh



5 cm mesh



Modelling by HSE – BE1 Unobstructed

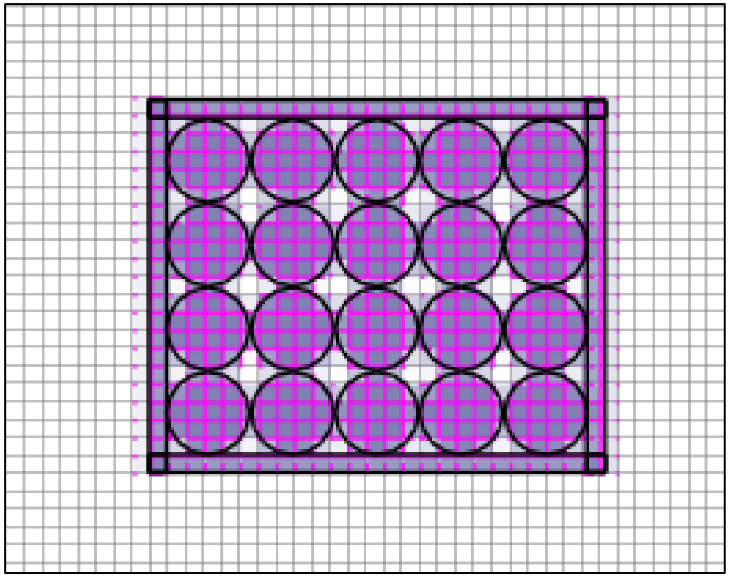


Mesh Size (cm)	20	10	5	2.5
Max. Pressure (barg)	0.027	0.016	0.043	0.057

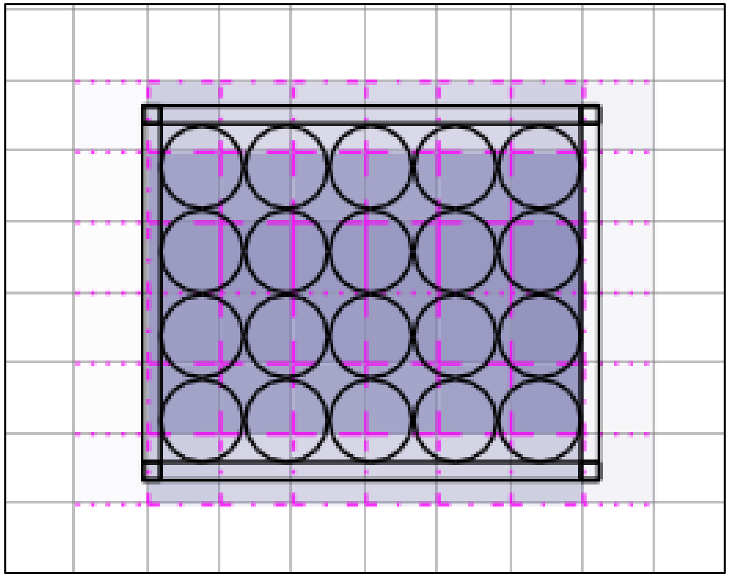
- Simulations show clear grid dependence
- Pressure traces different across all meshes
- Max. pressure in the container shows no trend with grid refinement
- Approx. factor of 2 difference in peak overpressure across mesh resolutions tested

Modelling by HSE – BE1 Obstructed

5 cm mesh



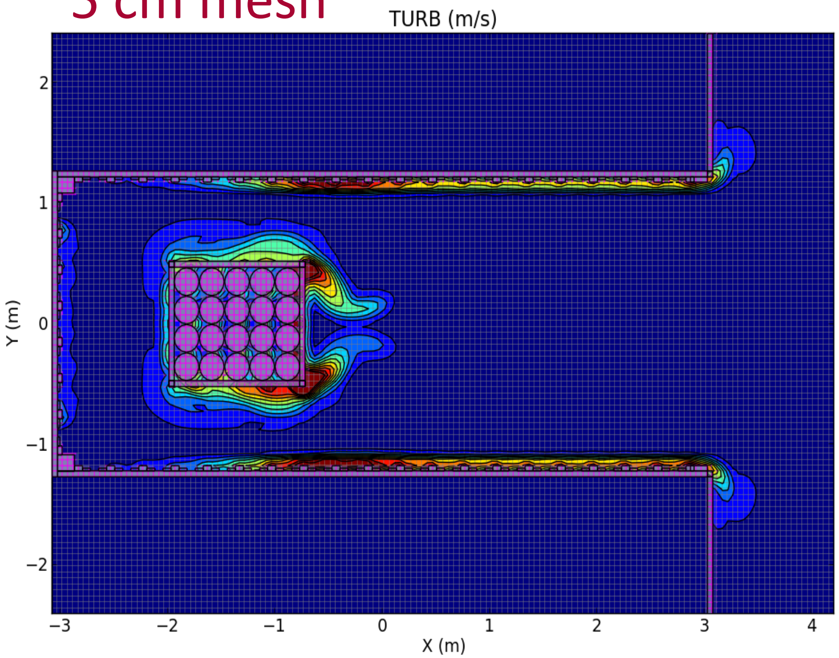
20 cm mesh



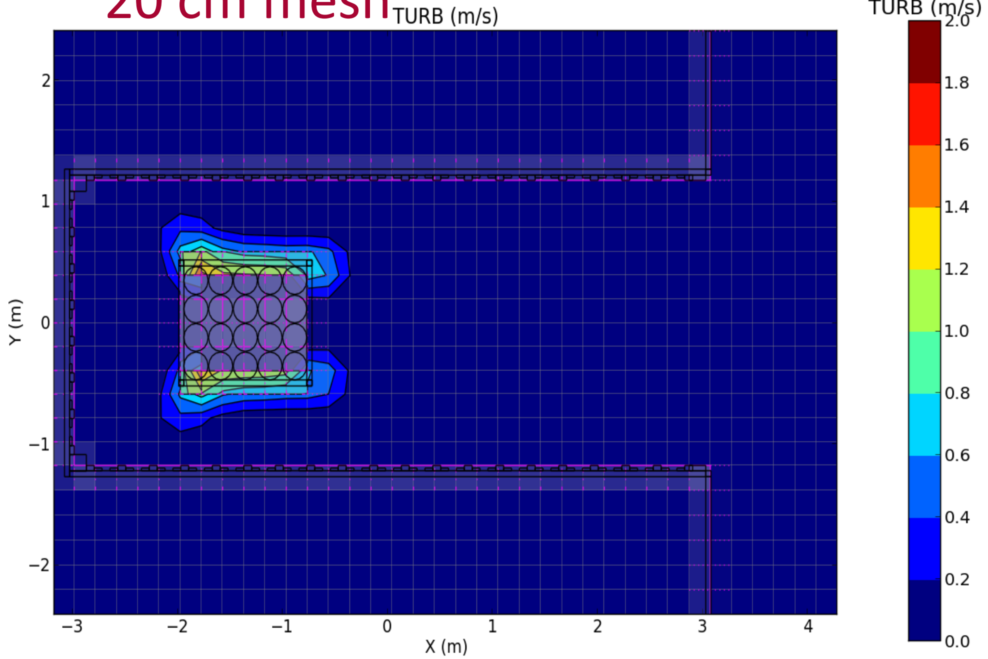
- Grid choice has a significant impact on geometry resolution
- FLACS porosity model intended to handle this by introduction of sub-grid-scale effects
- However, results show very different turbulence generation and explosion overpressures for the different meshes

Modelling by HSE – BE1 Obstructed

5 cm mesh

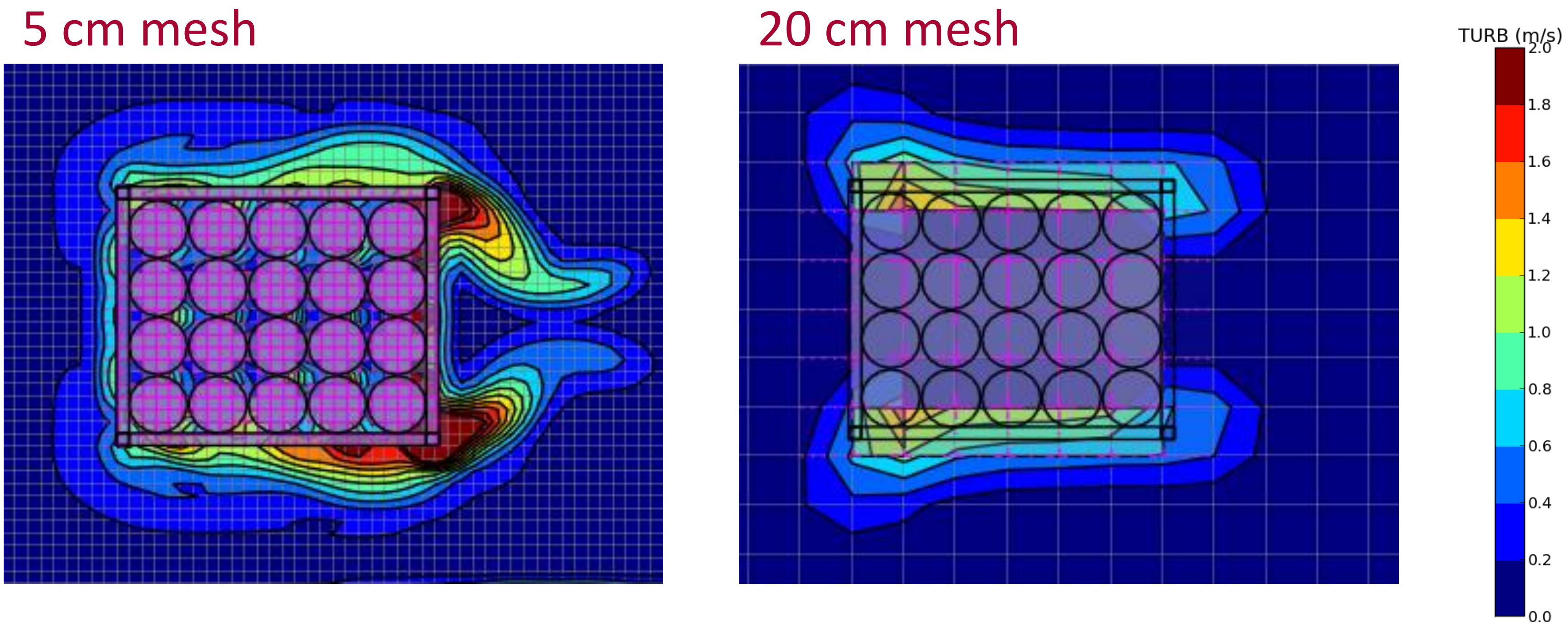


20 cm mesh



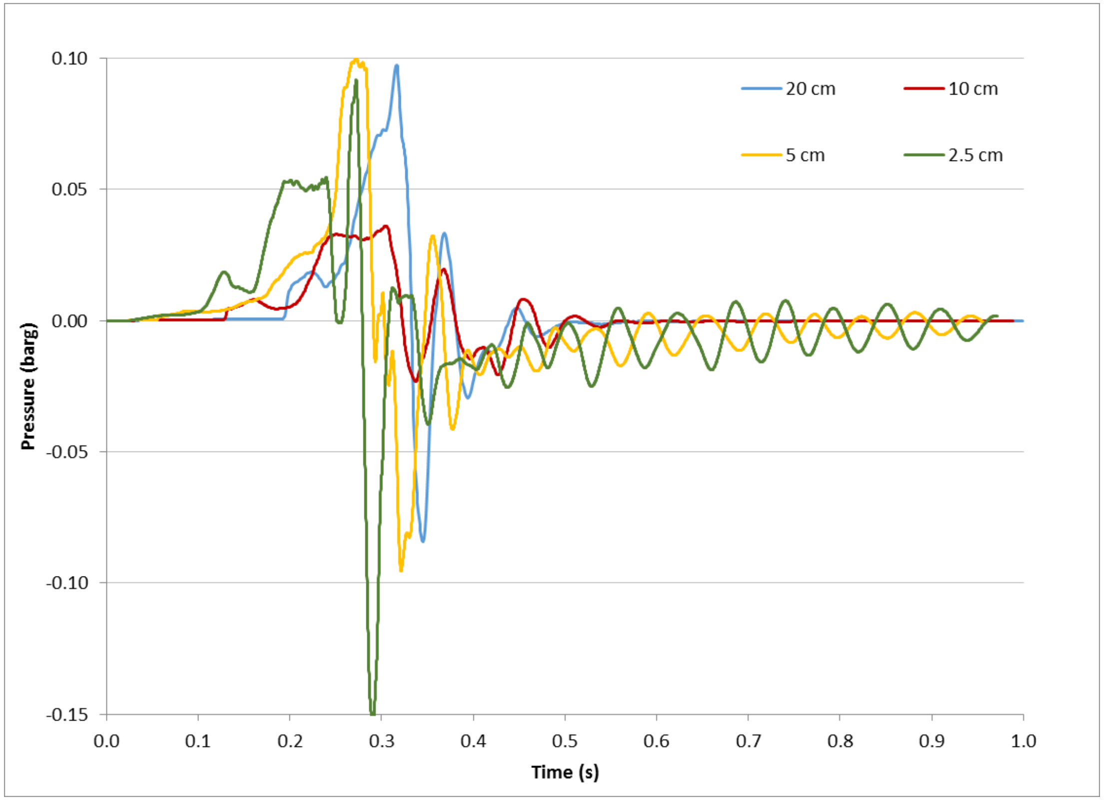
- Significant differences in turbulence generation at container walls (as before) and around bottle bundle obstruction

Modelling by HSE – BE1 Obstructed



- Higher turbulence velocities predicted around the cylinder bundle obstacle for the finer mesh

Modelling by HSE – BE1 Unobstructed

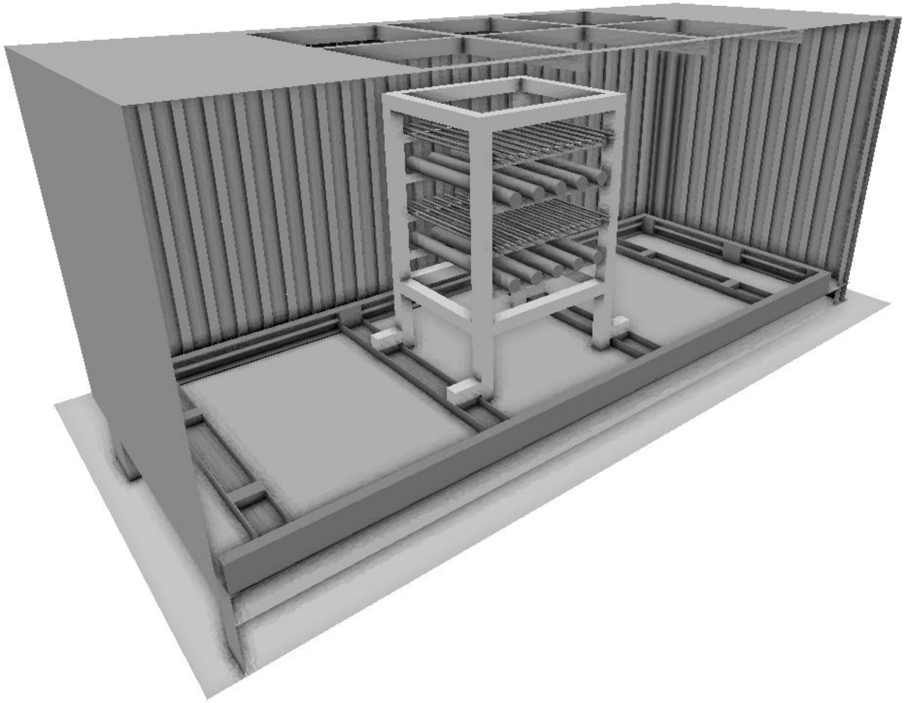


Mesh Size (cm)	20	10	5	2.5
Max. Pressure (barg)	0.101	0.036	0.106	0.092

- 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

Modelling by HSE – BE2

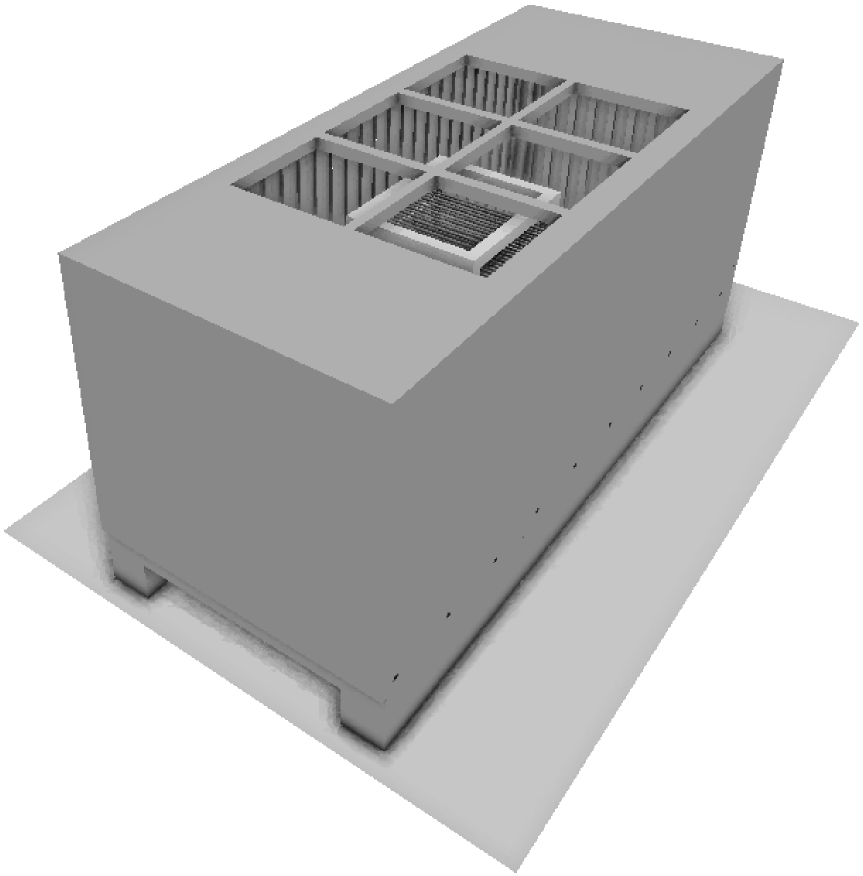
- Geometry for 2nd exercise is a slightly modified version of that used for the 1st blind-prediction study
- Again, geometry details are defined in the model in as much detail as possible



- 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

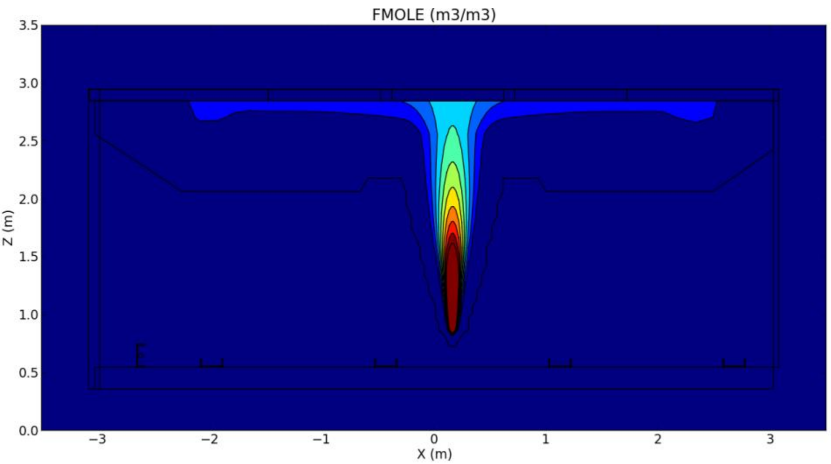
Modelling by HSE – BE2

- Additional features of geometry for the 2nd exercise include:
  - Closed container doors
  - Explosion vent panel openings in container ceiling
  - Holes along side of container to allow air to escape during H_2 jet release
- Corrugated walls remain crudely represented as was the case for the 1st blind prediction
- Differences in resolution of small geometrical features with different meshes remains, as does reliance on the FLACS porosity sub-model

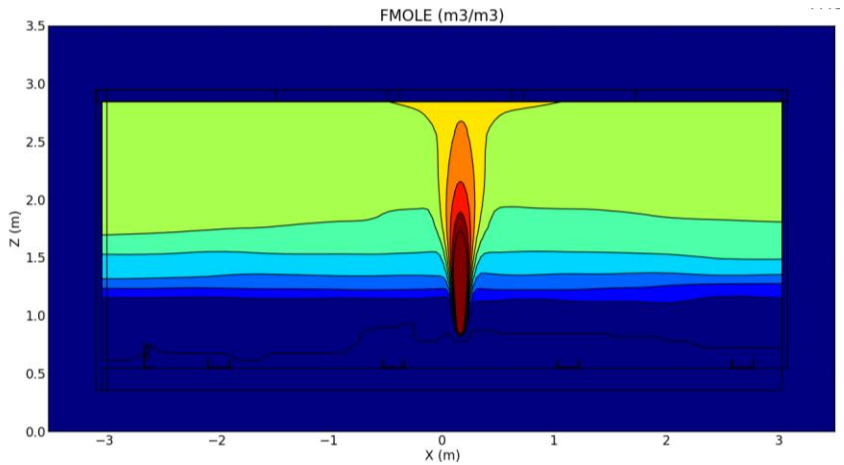


Modelling by HSE – BE2 Unobstructed

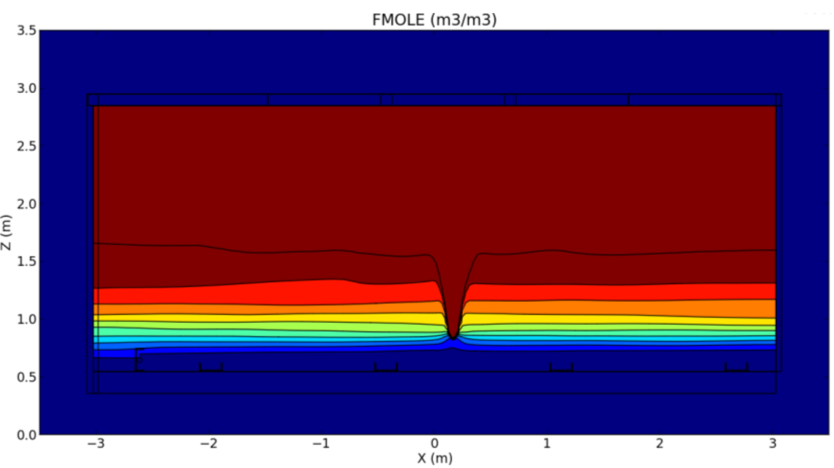
t = 10 s



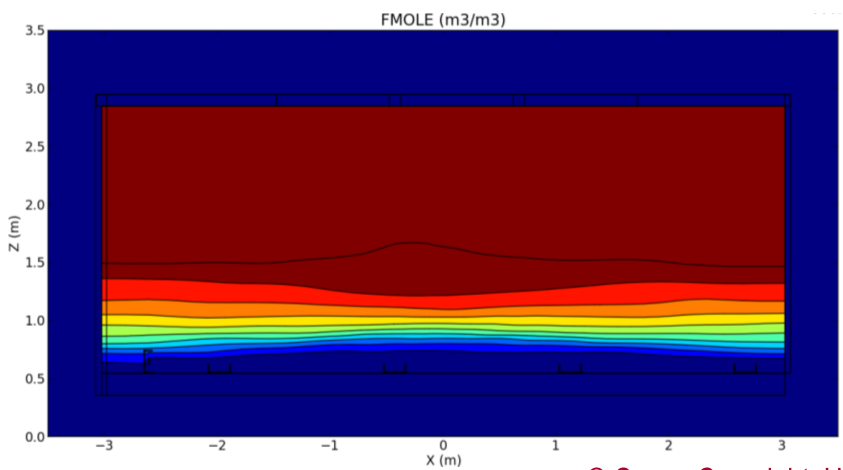
t = 180 s

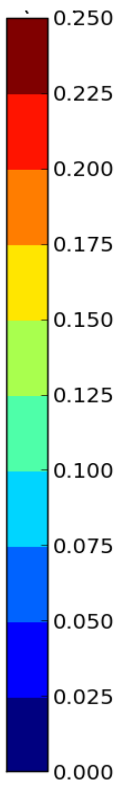


t = 450 s (end of H_2 release)

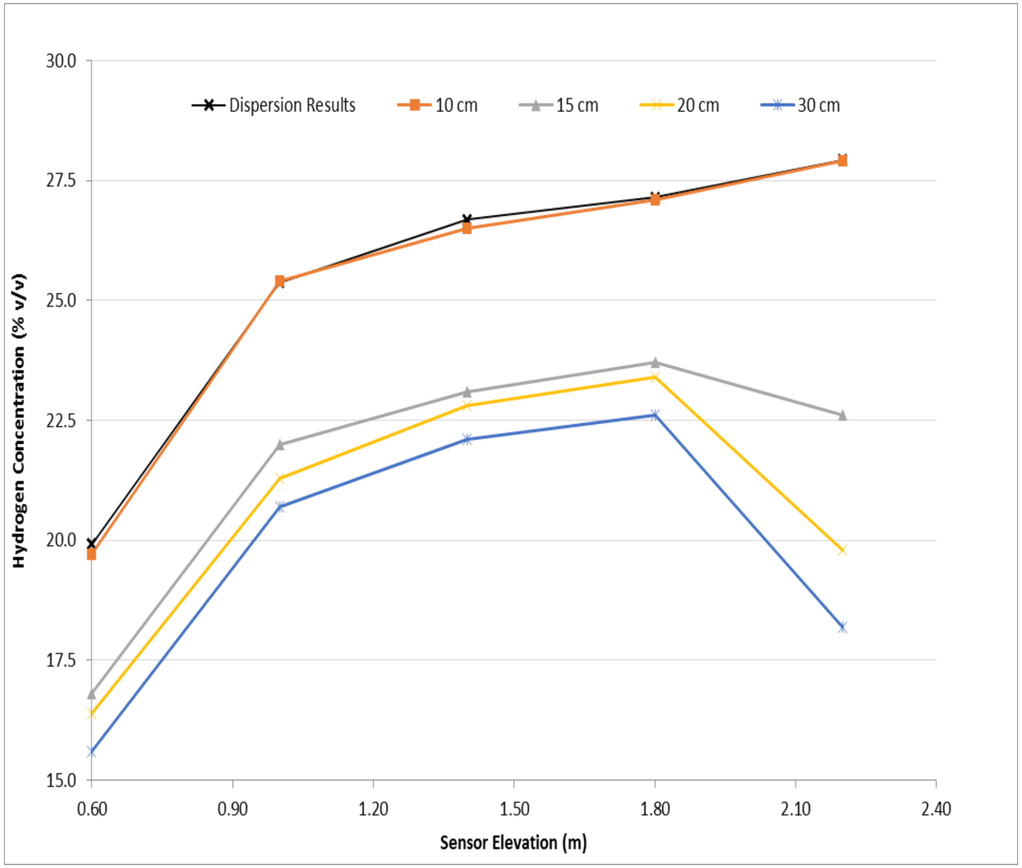


t = 480 s (time of ignition)





Modelling by HSE – BE2 Unobstructed



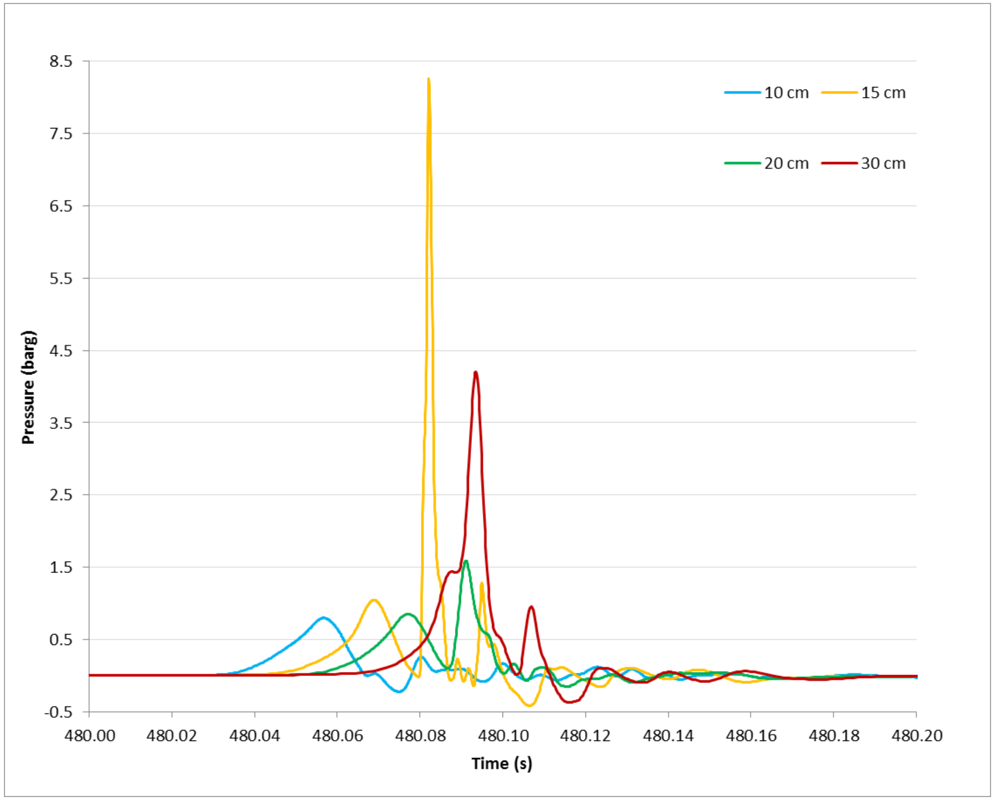
- Interpolated concentrations differ significantly across meshes
- Only the 10 cm mesh gives initial H_2 concentrations for the explosion simulation that are close to those at the end of the dispersion calculation
- This has a large influence on the resulting overpressures

Modelling by HSE – BE2 Unobstructed

Mesh Size (cm)	30	20	15	10
Max. Pressure (barg)	1.966	0.598	2.115	0.526

- 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

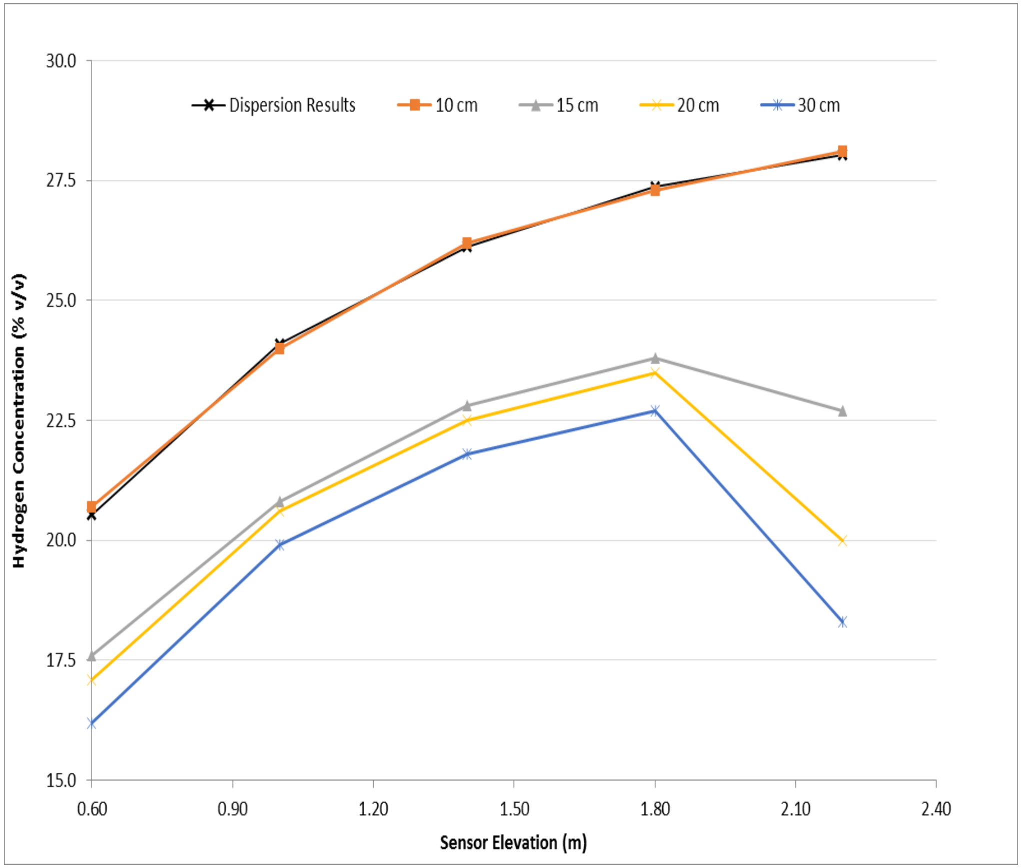
Modelling by HSE – BE2 Unobstructed



Mesh Size (cm)	30	20	15	10
Max. Pressure (barg)	4.201	1.591	8.266	0.798

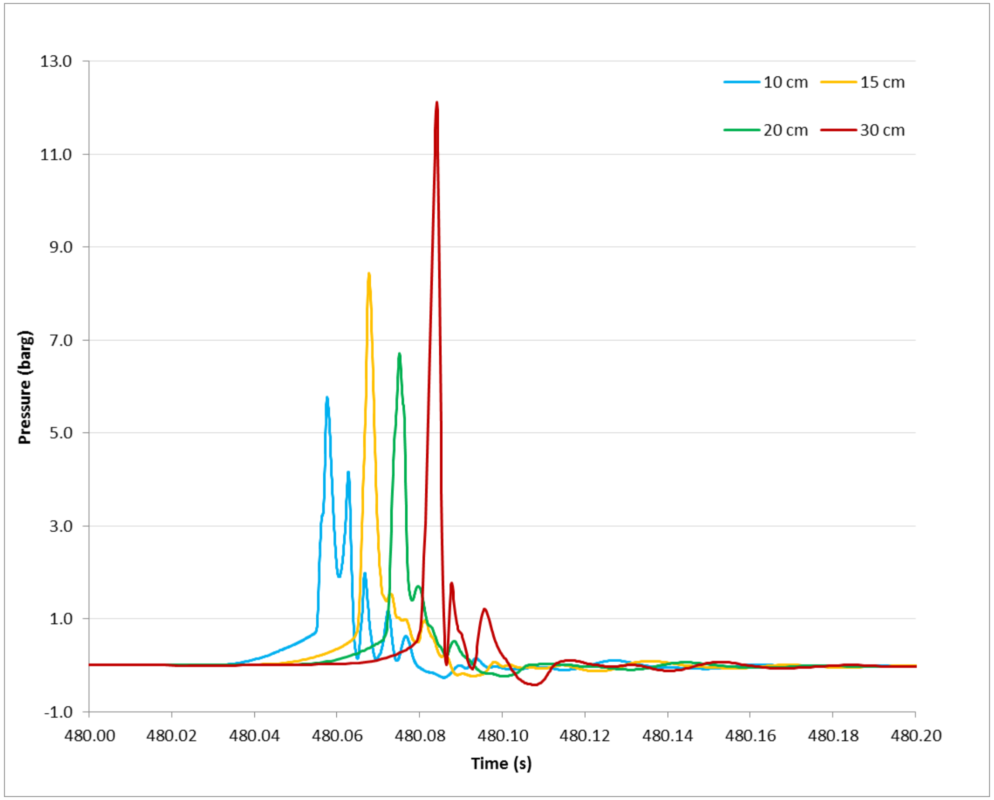
- Largest overpressures predicted at sensors furthest from ignition location (near opposite end of the ISO container)
- Again there are significant differences between the pressure traces predicted for different meshes
- Large variation in max. overpressure across mesh resolutions, with no trend observed

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



Mesh Size (cm)	30	20	15	10
Max. Pressure (barg)	12.12	6.72	8.44	5.77

- 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

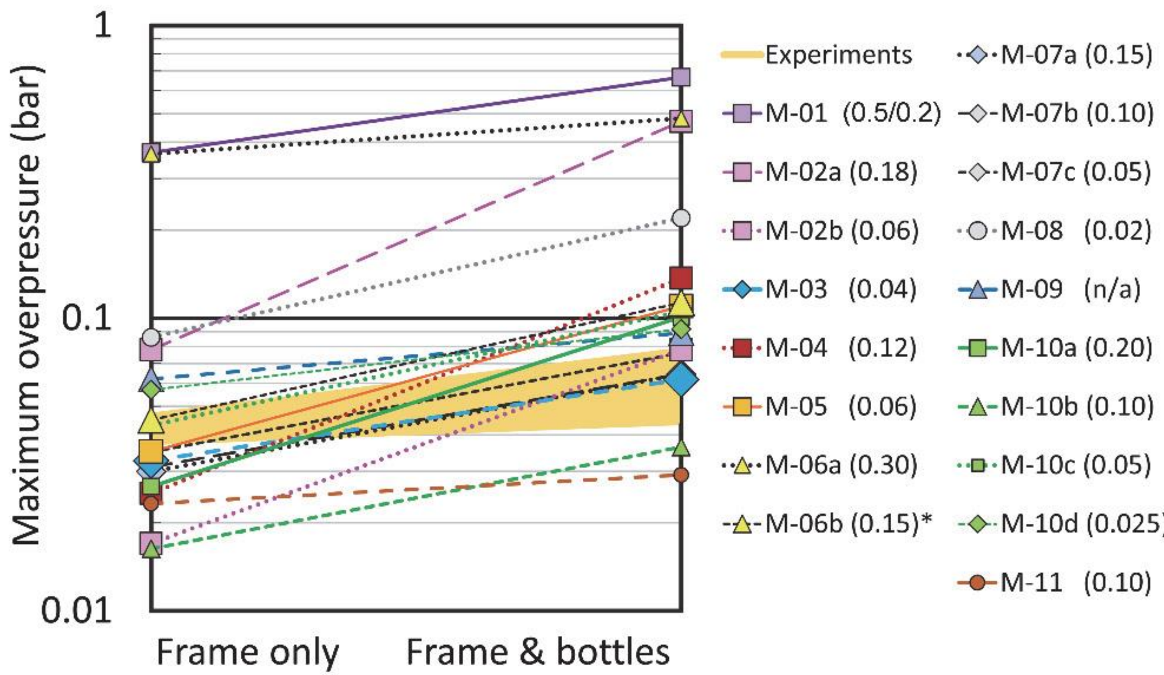


Figure taken from Skjold et al. (2017) [2]

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

[1] Skjold, T., van Wingerden, M., Enstad, G.A. and Carcassi, M. (2016), *HySEA – First blind-prediction study, Hydrogen explosions in ISO containers with homogeneous mixtures*, 3rd Announcement, HySEA-D-4-05-2015 Rev. 03, GexCon

[2] Skjold, T., et al. (2017), Blind-prediction: Estimating the consequences of vented hydrogen deflagrations for homogeneous mixtures in 20-foot ISO containers, *International Conference on Hydrogen Safety,* 11-13 September 2017, Hamburg, Germany

Questions?