UK EXPLOSION LIAISON GROUP

35th Anniversary Meeting
Spadeadam, 10-12 October 2017

A review of CFD for simulating hydrogen explosions, and how to improve confidence in the approach

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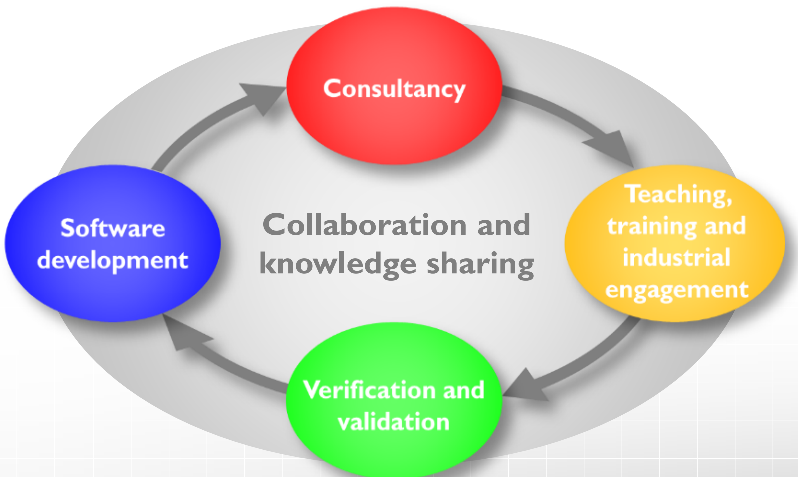

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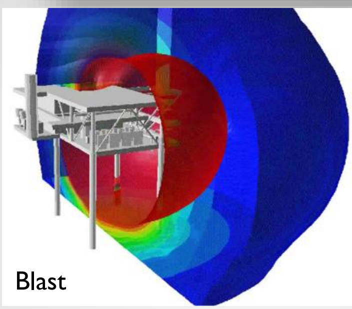
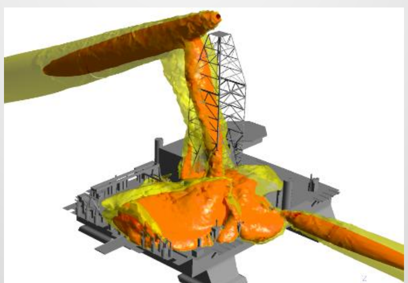
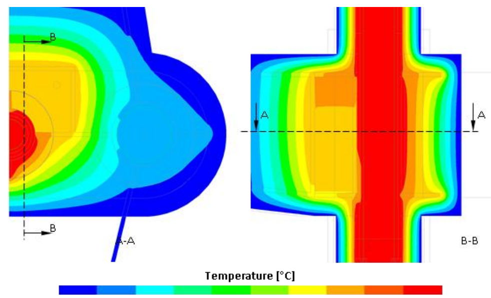
Technical safety

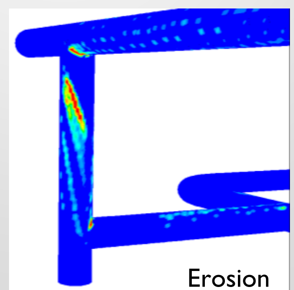

Blast


Deepwater Horizon : http://abercus.com/News_20110622.aspx

Flow assurance

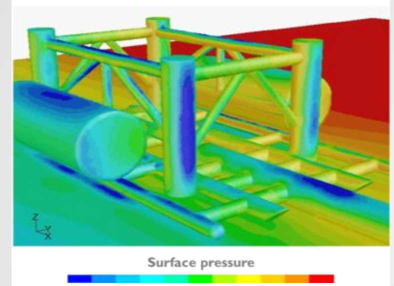
Hydrate avoidance

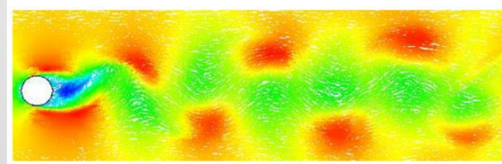



Erosion

Subsea engineering

Subsea stability




Flow induced vibration

Agenda

- Background and introduction
- Modelling and simulation
- Application of computational fluid dynamics
- Validation and consistency across industry
- Explosion risk analysis
- Probabilistic structural response
- Summary

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Background and introduction

- Hydrogen explosions are quite different from those for conventional fuels
  - buoyancy will quickly remove accumulated hydrogen when unconfined
  - the flammable range is wider
    (LFL is not so different)
  - hydrogen is more reactive
    (~ ten times more reactive than natural gas)
  - a hydrogen deflagration is more likely to transition to detonation
  - lower energies are needed to ignite hydrogen
    (~ one-tenth of that for gasoline vapours)
  - the J-T coefficient for hydrogen is negative, so a leaking gas *warms*, which increases the likelihood of spontaneous ignition.

Background and introduction

- Hydrogen safety issues are a crucial aspect for wide spread deployment and use of hydrogen and fuel cell technologies
- Because of the greater potential hazards, hydrogen technologies typically need additional mitigation when compared to conventional fossil fuel technologies
- There have been a number of joint R&D projects – HySafe, IEA Task 19/31/37, HyIndoor, NaturalHy, HySEA, SUSANA, …
- Further research and development leading to practical good practice guidance for reliable analysis is required.

Background and introduction

Hydrogen combustion accidents

Hindenburg 1937

Porsgrunn 1985

Fukushima 2011

Most accidents involving hydrogen combustion are catastrophic – perhaps because of transition to detonation

Background and introduction

Industrial accident conditions

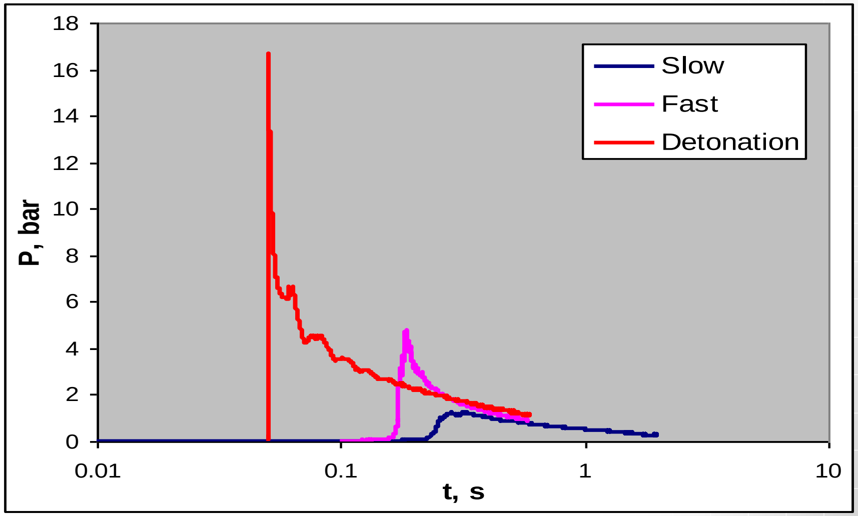
- Various hydrogen-air mixture compositions (4% - 75%)
- Various geometries and environment
  - open geometry: outside buildings, little influence of partial confinement and obstacles (in containment such as dome area)
  - partially confined: limitation in space or geometry; near walls, roofs…
  - confined explosions inside rooms, compartments, pipes…
- Various congestion
  - high: extensive blockage by pipework, cabling, repeating obstacles…
  - medium: intermediate level of space obstruction
  - low: open space with little blockage of the flame propagation path
- Ignition source.

Background and introduction

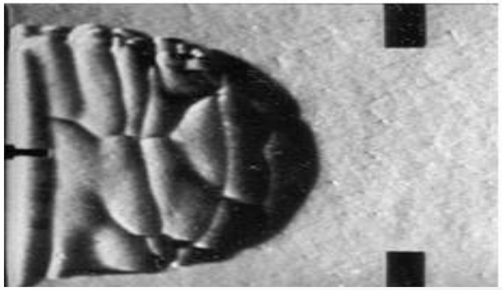
Flame propagation regimes

Combustion regime is important for the determination of pressure loads

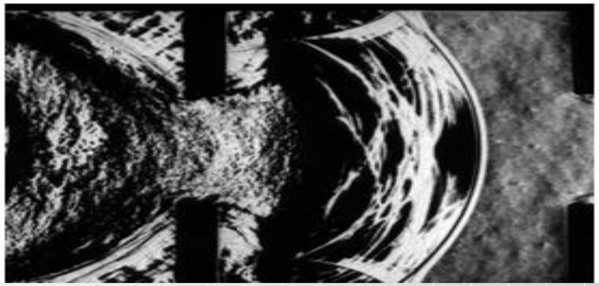
- slow flame
- turbulent flame
- fast turbulent flame
- DDT
- detonation.



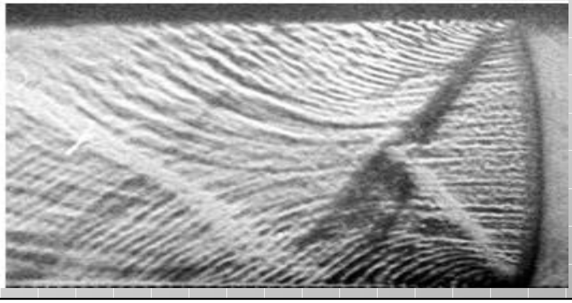
Slow subsonic flame



Fast subsonic flame



Detonation

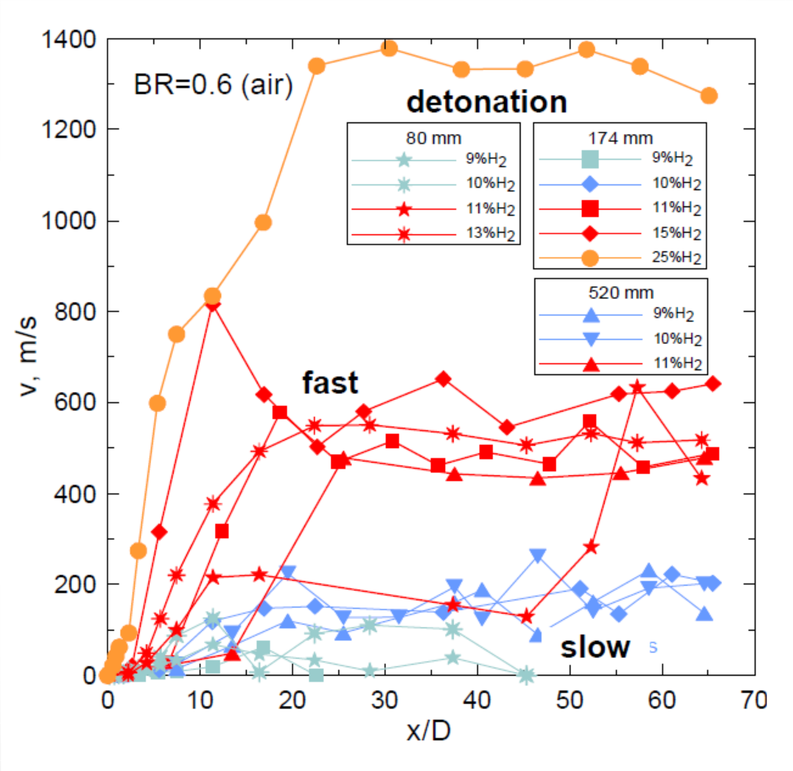


Background and introduction

Possible combustion regimes during an accident

With respect to the speed of sound in the products C_{sp}, three different regimes can be distinguished:

- slow deflagration ($v < C_{sp}$)
- fast deflagration ($v \sim C_{sp}$)
- detonation ($v \sim 2\ C_{sp}$)



Flame speed along combustion tube
different tube configurations and mixture compositions

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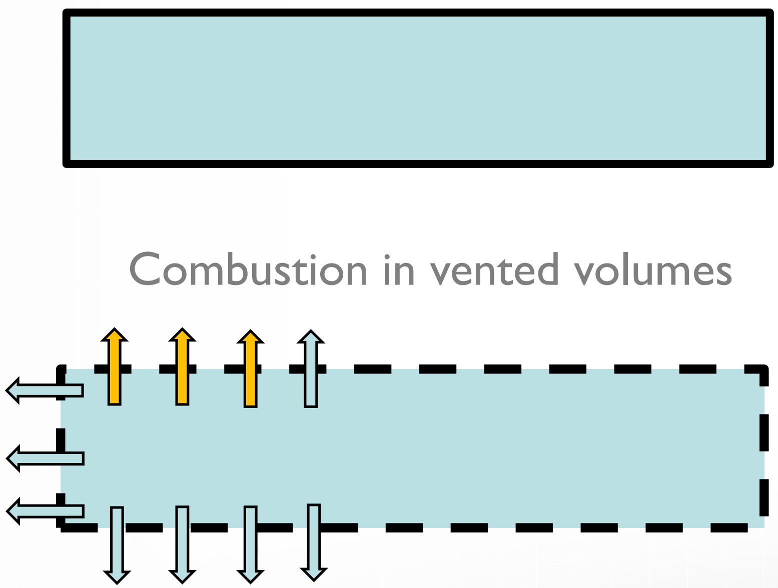
Modelling and simulation

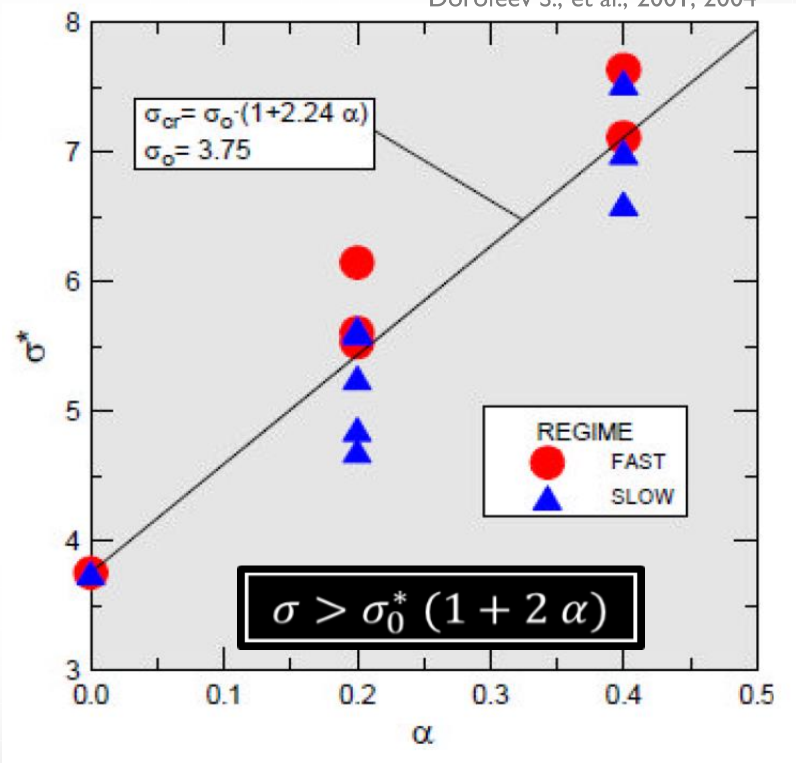
Flame acceleration criterion (vented combustion)

Alekseev V., et al., 2000
Dorofeev S., et al., 2001, 2004

Combustion in closed volumes

Combustion in vented volumes





Dependence of the critical expansion ratio on vent ratio

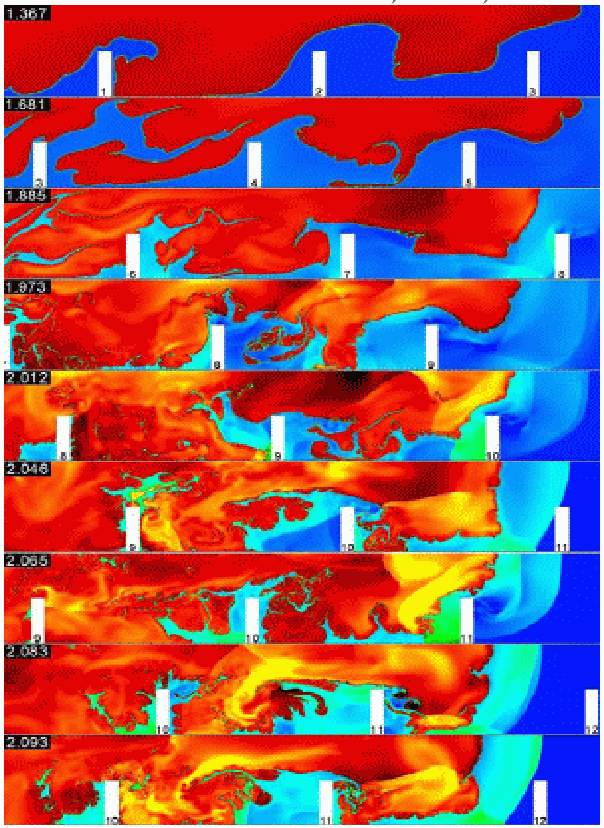
Modelling and simulation

Detailed modelling of flame acceleration and DDT

Requires high enough resolution for chemistry and turbulence, including:

- reproduction of the interaction of generated acoustic waves with flame
- multiple reflections from obstacles and walls
- possible development of powerful instabilities such as Kelvin-Helmholtz and Richtmyer-Meshkov

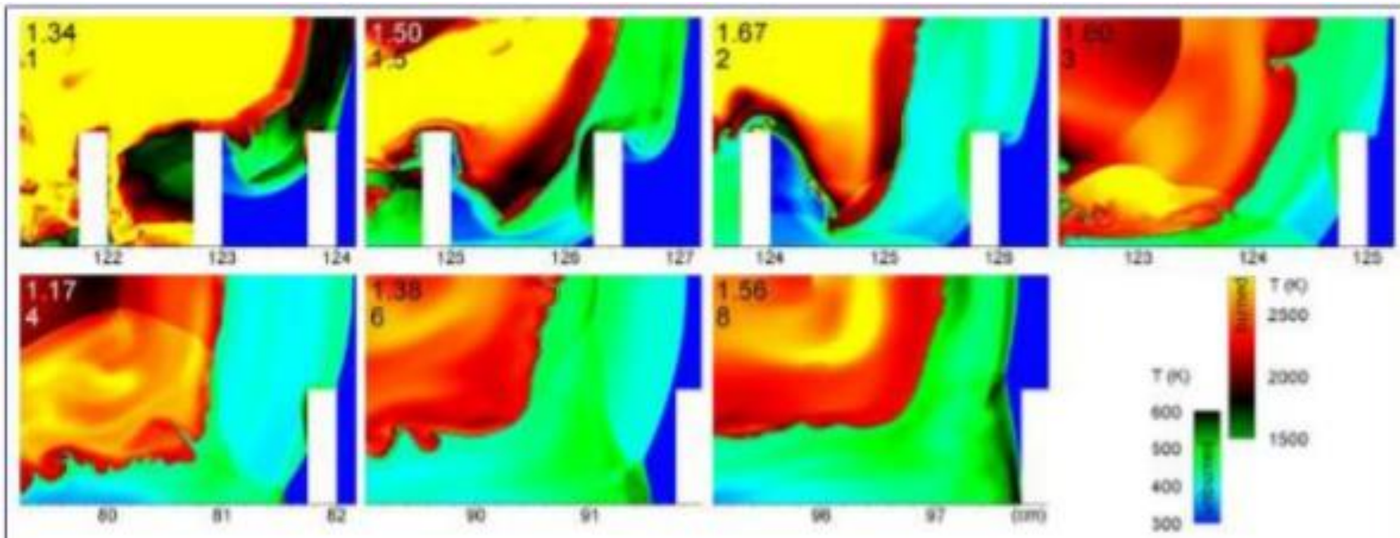
Gamezo, et al, 2007



Modelling and simulation

Detailed modelling of flame acceleration and DDT

- Need very fine spatial grid and timesteps to capture important physics at the flame
- Whilst this represents important progress, this is not a practical, fit for purpose approach for design.



Gamezo, et al, 2007

Modelling and simulation

Practical needs

- Whilst the principles of combustion and detonation processes are reasonable well understood, the prediction of the distinct flame propagation regime remains a challenging task
- The safety engineer needs to know which combustion regime is to be expected
- The technical recipes often used can be subjective or even not fully consistent:
  - LFL and UFL for combustion possibility
  - concentration limits for explosion / detonation possibility
  - evaluation of the combustion speed in comparison with sound speed as criterion for transition to detonation

Modelling and simulation

Practical needs

- Following numerous scientific studies on flame acceleration and DDT, we still do not have a complete understanding of these complicated events
  - stochastic nature complicates their confident prediction both in the experiments and in detailed CFD simulations
- Industry needs a methodology based on the evaluation of the possibility for flame acceleration and DDT depending upon the basic engineering characteristics of the system, such as geometrical properties and composition of the mixture
- CFD analysis is a practical, yet accurate approach.

Agenda

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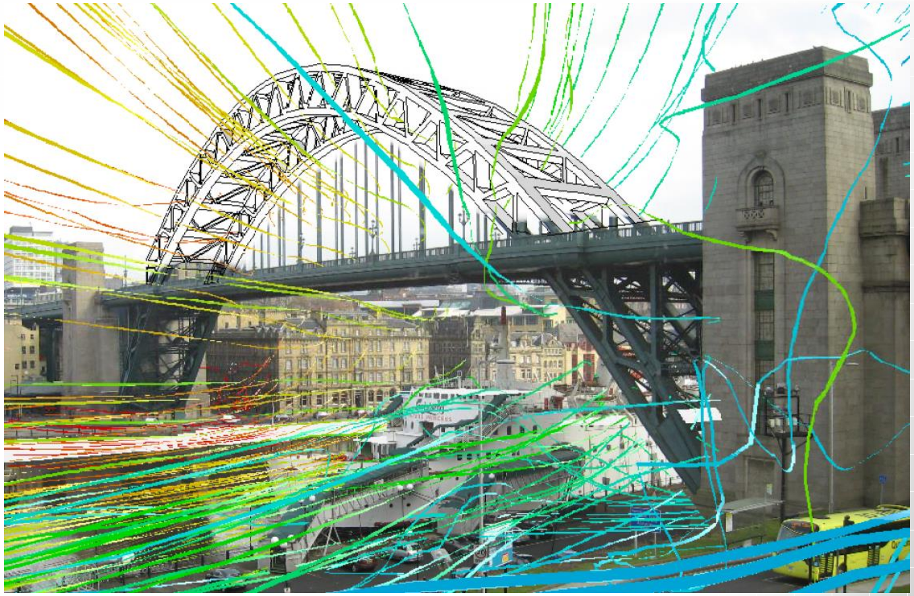
Application of computational fluid dynamics

What is CFD?

Models that simulate real life processes:

- realistic representation of the geometry of interest
- solving the fundamental physical equations
- conservation of mass, momentum and energy
- utilization of fundamental chemical properties for the components involved.



Application of computational fluid dynamics

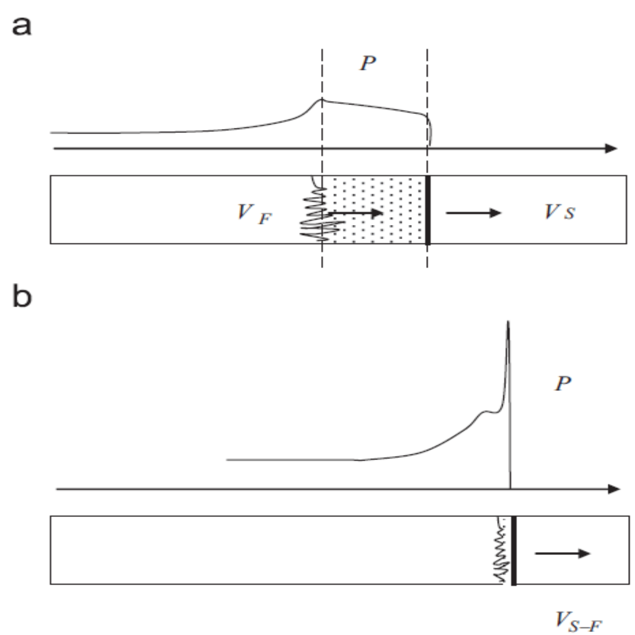
Available CFD tools

- General purpose CFD codes
  - simulate hydrogen explosions in theory but are not fit for purpose for design purposes due to the computational overhead associated with the refined mesh and time step required
- Explosion-specific CFD codes (FLACS, EXSIM, …)
  - utilize physical sub-models for combustion processes which allows a coarser discretization to be used
  - a practical, fit-for-purpose approach for design
- Other non-commercial tools
  - (COM3D, REACFLOW)
- Verification and validation is generally very important!

Application of computational fluid dynamics

Prediction of DDT – CFD approach

- DDT likelihood is illustrated by the spatial pressure gradient across flame front (Middha & Hansen, 2006-08)

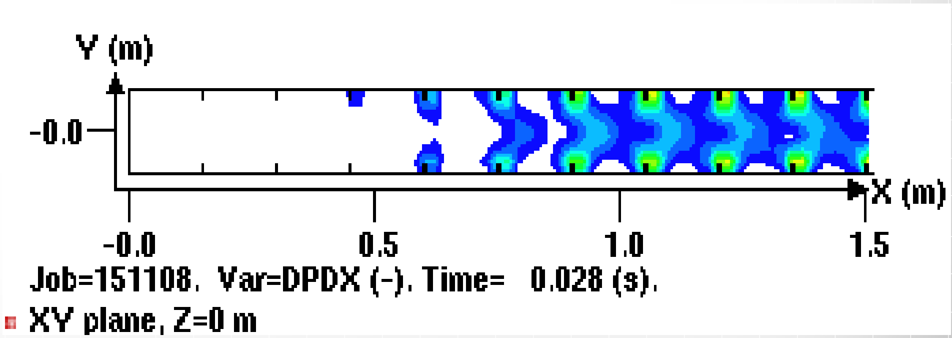


$$\left.\frac{dP}{dx}\right|_{normalized} = \left.\frac{dP}{dx}\right|_{actual} \frac{X_{CV}}{P_0}$$

Application of computational fluid dynamics

Prediction of DDT – CFD approach

- DPDX plots combined with plots comparing geometrical dimension with detonation *cell size*
- Description of DDT by CFD an *engineering* approach
- Validation carried out against several practical systems
  - Sandia FLAME facility
  - detonation tubes (McGill)
  - LANE geometry (FhICT)
  - ...

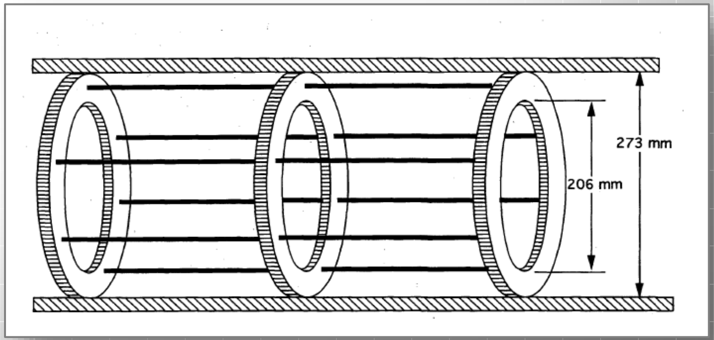


Middha & Hansen (2006-08)

Application of computational fluid dynamics

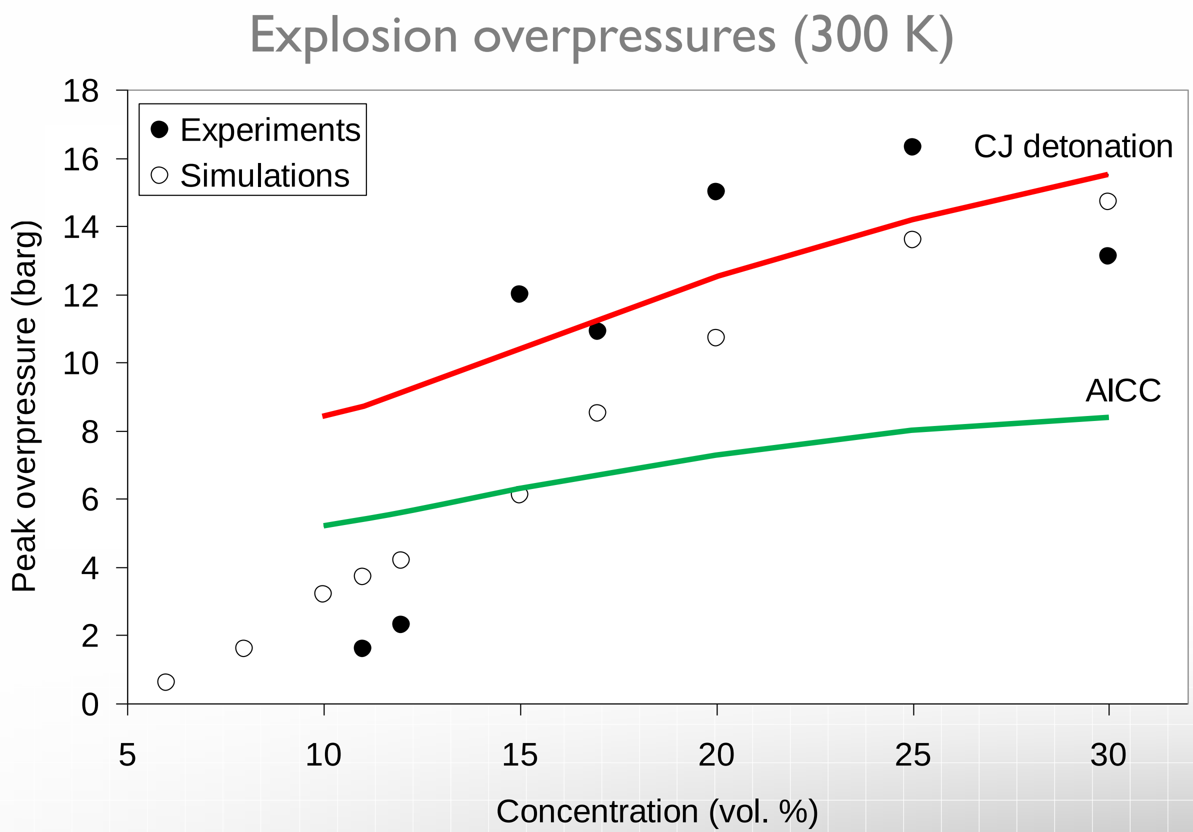
Brookhaven HTCF study

- The experiments are carried out in a heated detonation tube with an array of orifice plate obstacles placed along the tube
  - the tube is 21.3 m long and has an internal diameter of 273 mm
  - the orifice diameter is 206 mm (equivalent to a blockage ratio of 43%)
  - the spacing between neighbouring orifice plates is 273 mm
- Combustion of premixed hydrogen-air mixtures at various concentrations are considered
- Ignition is at the closed end of the tube
- Three different starting temperature are considered: 300 K, 500 K and 650 K.



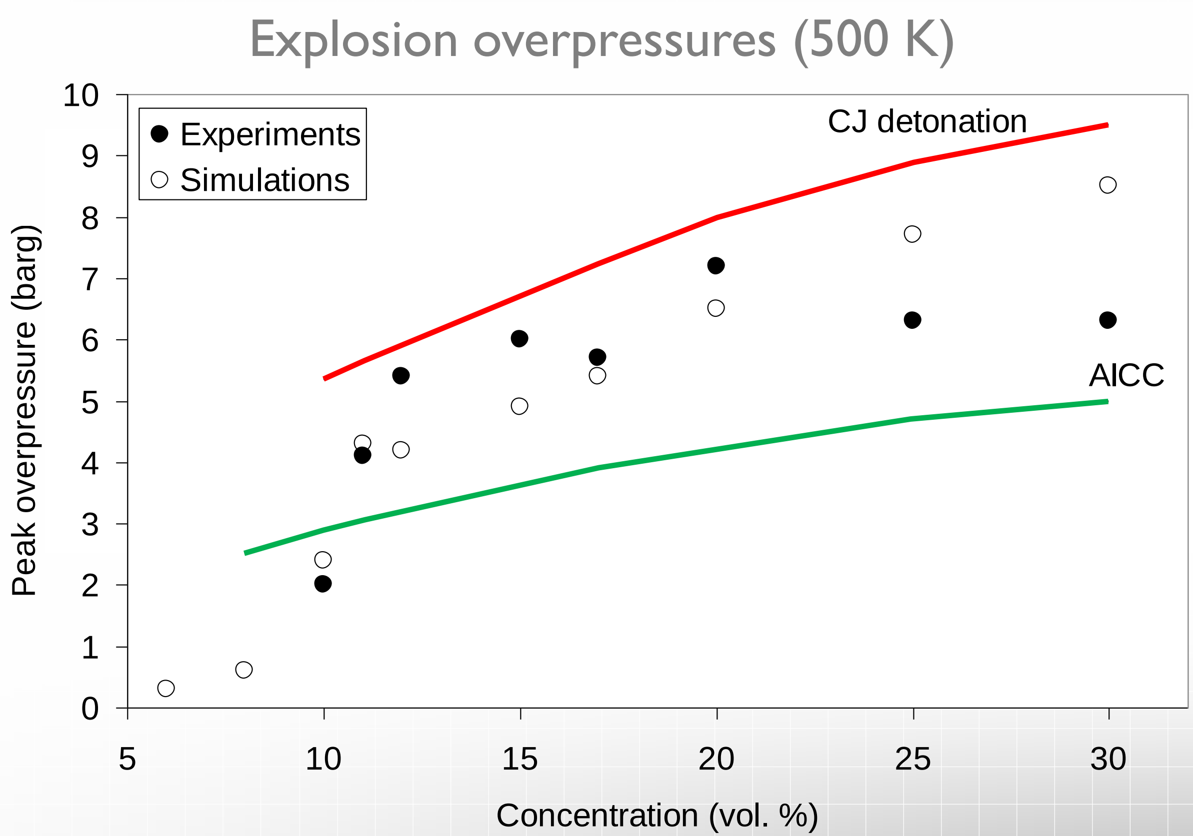
Application of computational fluid dynamics

Brookhaven HTCF study



Application of computational fluid dynamics

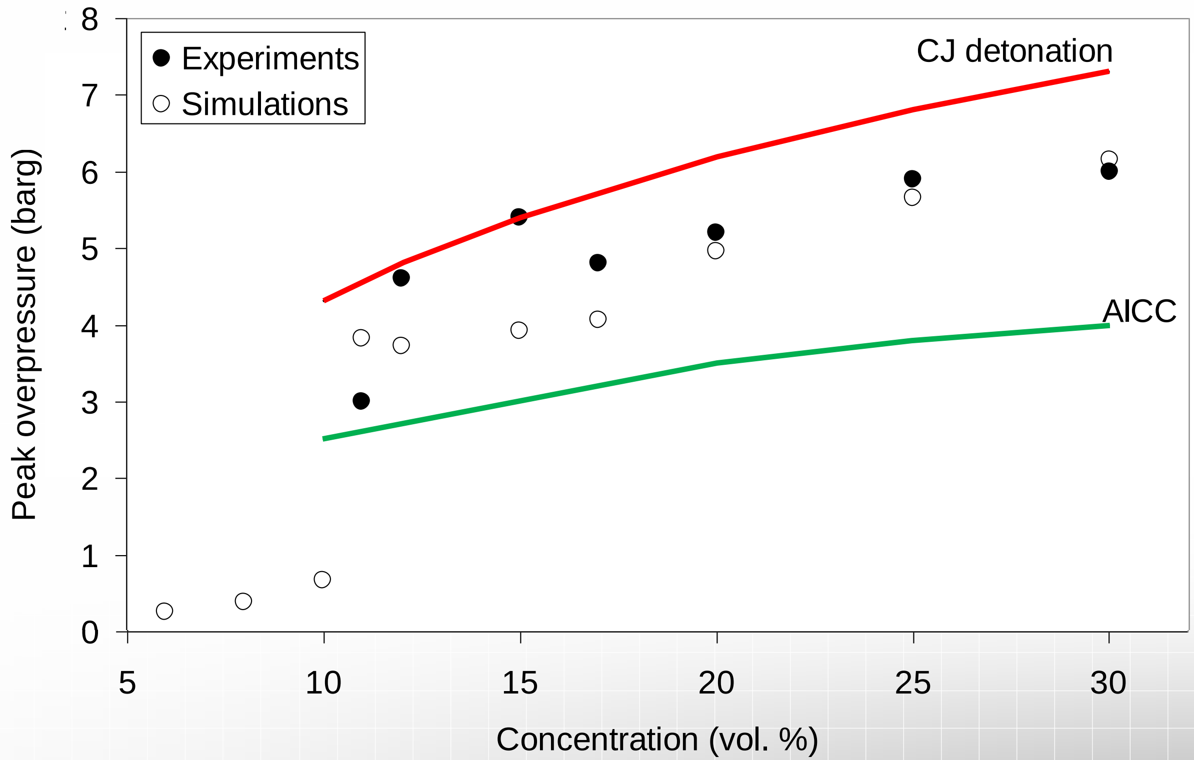
Brookhaven HTCF study



Application of computational fluid dynamics

Brookhaven HTCF study

Explosion overpressures (650 K)



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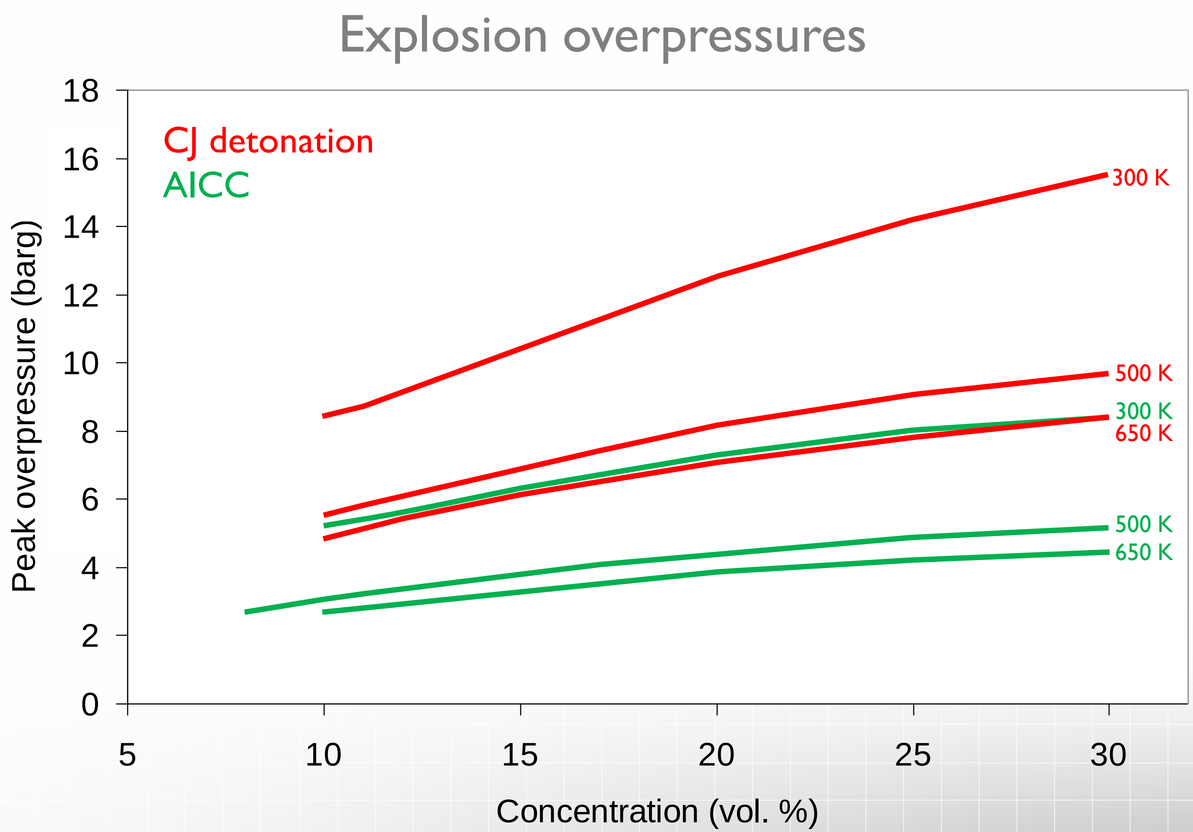
Application of computational fluid dynamics

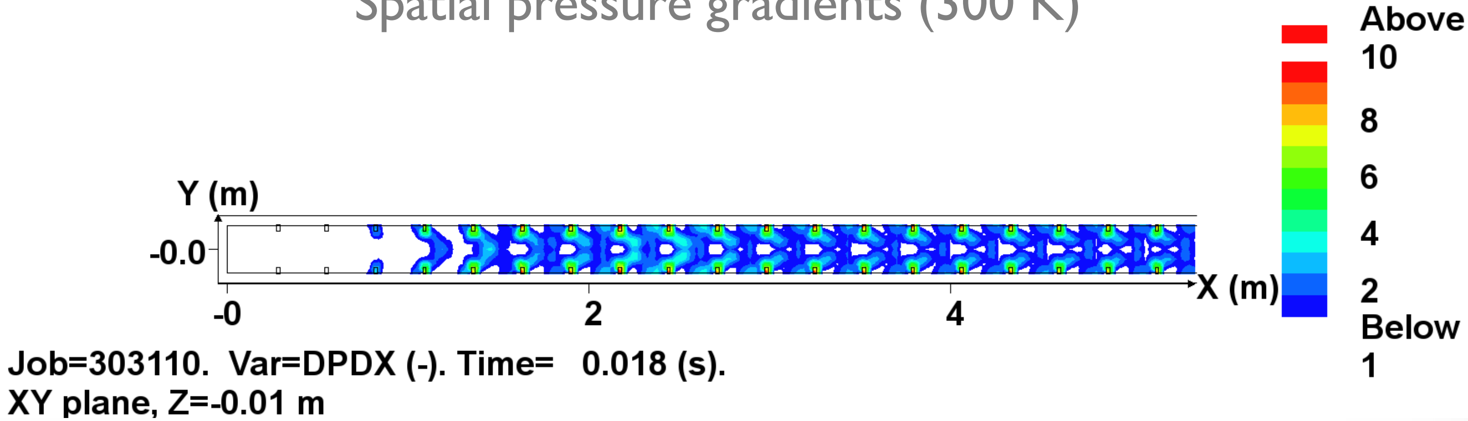
Brookhaven HTCF study



Application of computational fluid dynamics

Brookhaven HTCF study

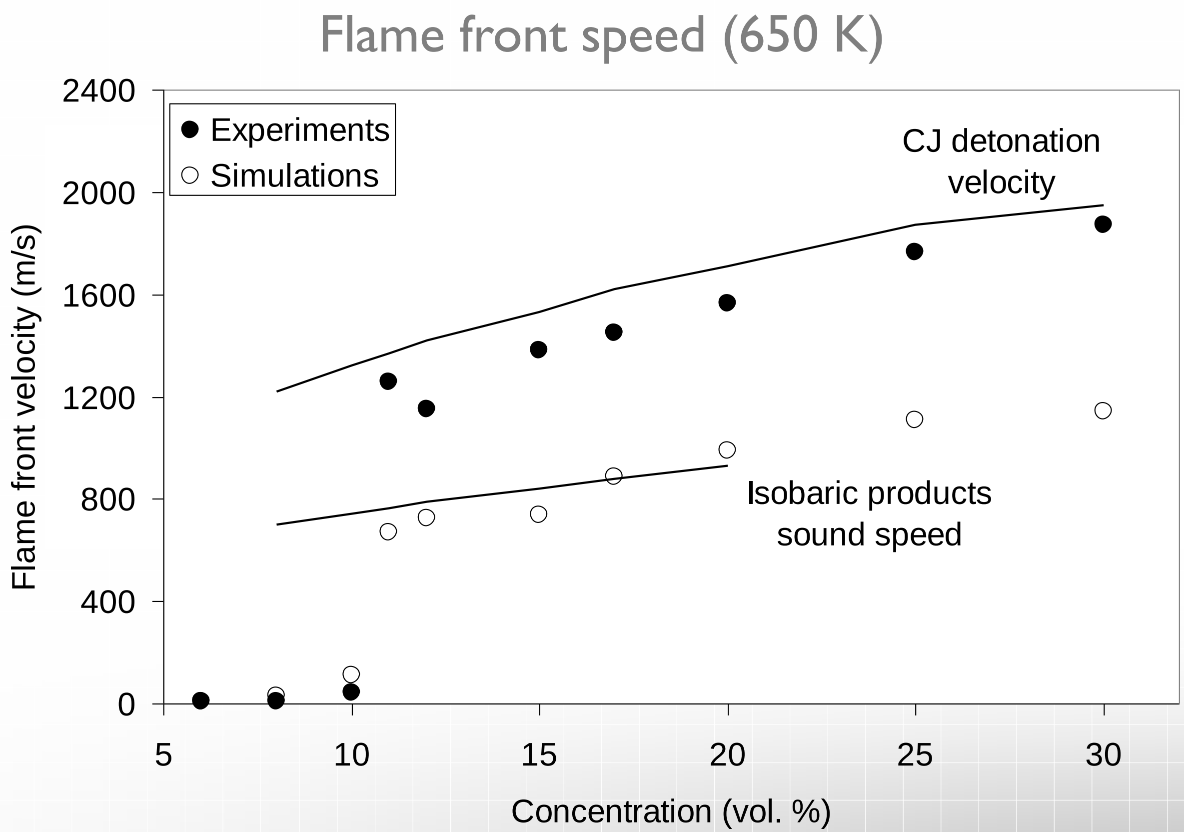
Spatial pressure gradients (300 K)



Simulations are unable to predict the exact run-up distance to detonation, but the location can be indicated as that where significant pressure gradients occur.

Application of computational fluid dynamics

Brookhaven HTCF study

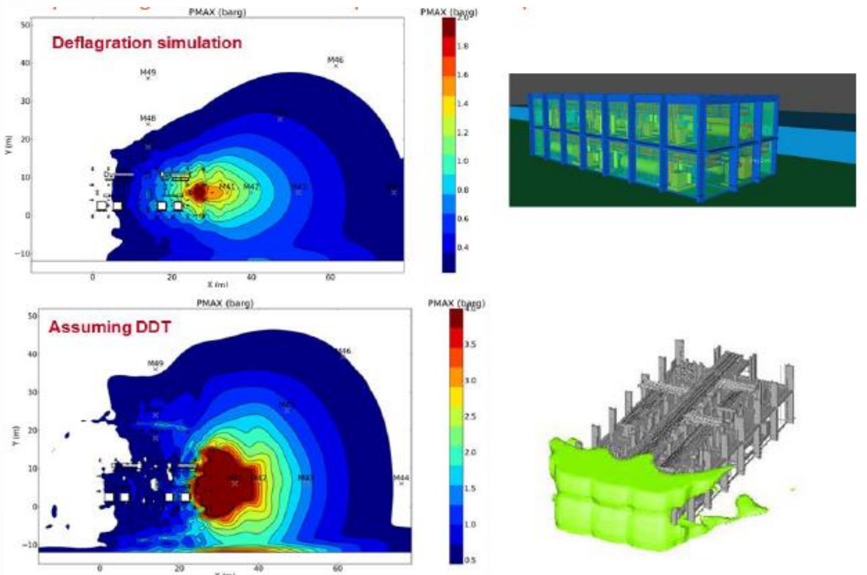


Application of computational fluid dynamics

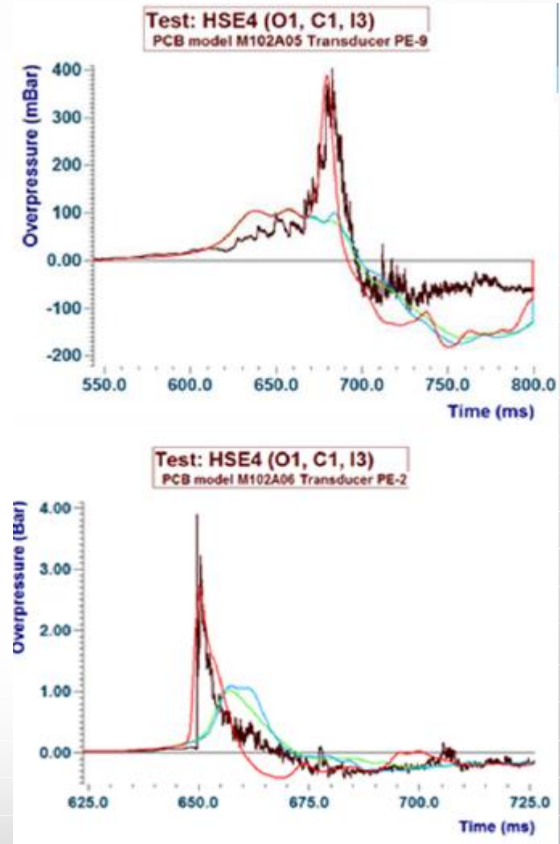
DDT simulations

DDT has been simulated using CFD (RANS) by some practitioners, but this is not yet commonplace

– (FLACS – HSE tests with natural gas).



Hansen & Johnson (2013)



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Validation and consistency across industry

Confidence in CFD

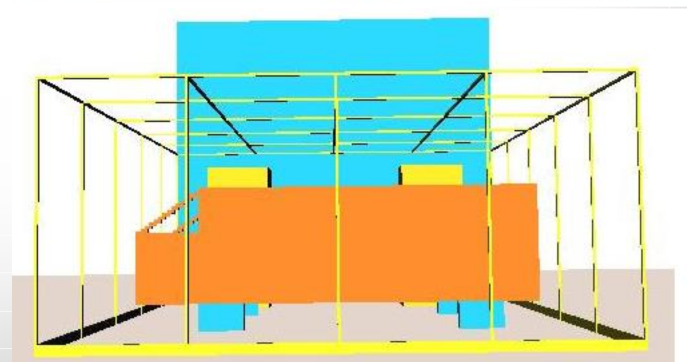
- CFD is increasingly used to perform safety analysis of potential accident scenarios (production, storage, distribution)
- Whilst CFD is a powerful numerical tool, it requires a high level of competence and knowledge to be used in meaningfully
- To improve confidence in CFD and on the accuracy of the simulation results, two main issues have to be addressed:
  - the capability of the CFD models to accurately describe the relevant physical phenomena
  - the capability of the CFD users to follow the correct modelling strategy
- The reliability/accuracy of CFD remains a significant concern – **blind benchmarking exercises** can help to demonstrate this.

Validation and consistency across industry

Blind benchmarking – hydrogen refuelling station (2007)

Reference needed

- An experimental mock-up of a hydrogen refuelling station was created by Shell and HSL, incorporating 2 dispensers and 1 vehicle
- Blind simulations were undertaken by several respected parties for a hydrogen explosion (homogeneous, stoichiometric hydrogen-air cloud with a volume of 90 m^3).

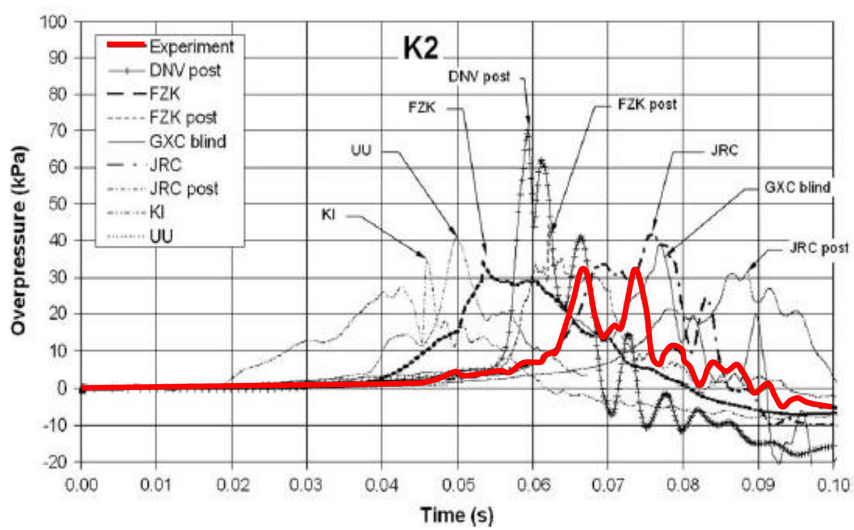


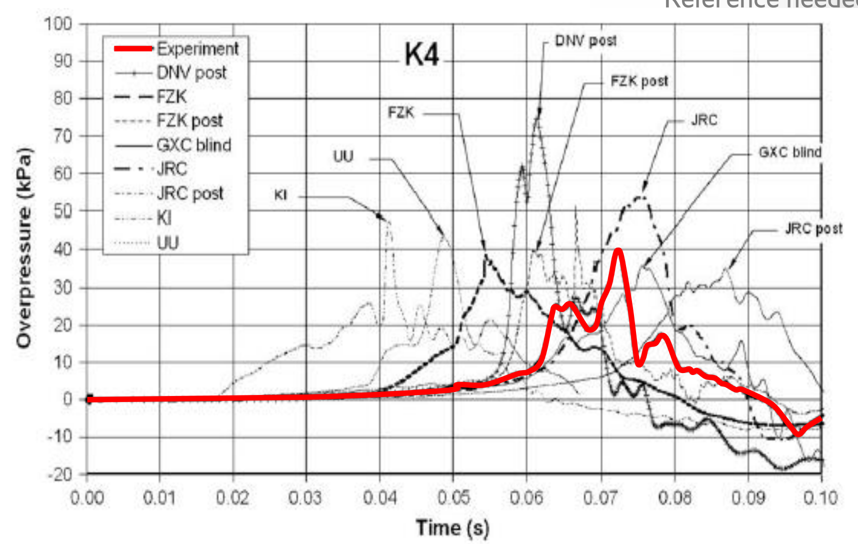
Validation and consistency across industry

Blind benchmarking – hydrogen refuelling station (2007)

- A comparison of the measured and simulated overpressure at two measuring locations, K2 and K4, is shown below
- There are discrepancies and scatter among the predictions.

Reference needed





Validation and consistency across industry

Blind benchmarking – HySEA experiments (2017)

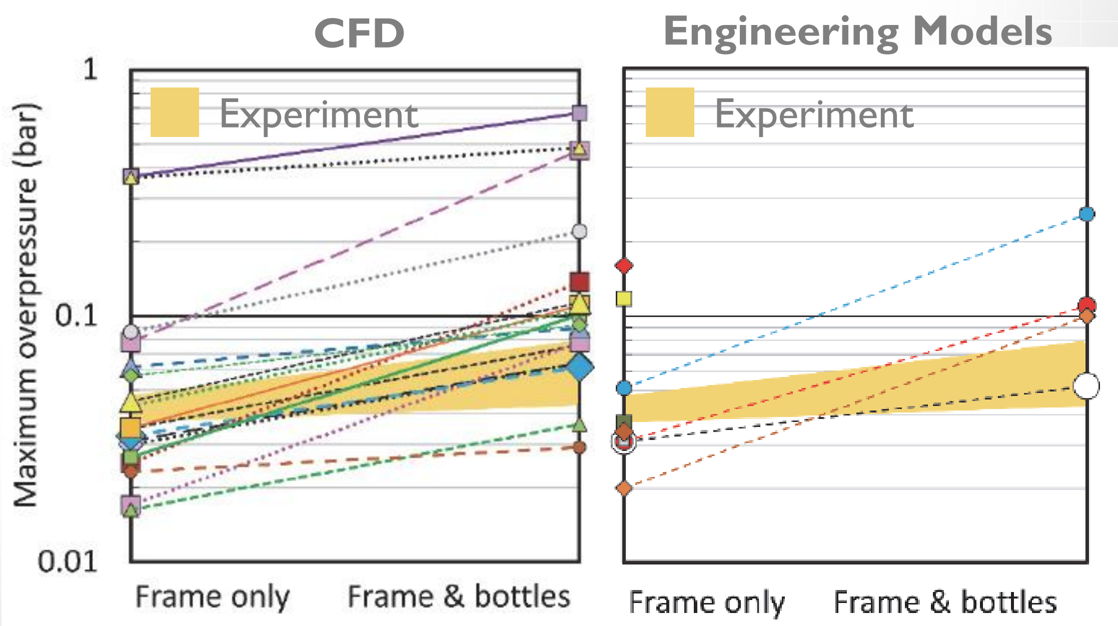
- The HySEA project has considered vented hydrogen deflagrations inside 20-ft ISO containers, both with and without internal obstacles
- Blind simulations have been undertaken by several parties for two scenarios (frame only, and frame plus bottles) for a homogeneous hydrogen-air mixture
- A comparison of the measured and simulated maximum overpressure within the container is shown overleaf.

Skjold, et al, 2017

Validation and consistency across industry

Blind benchmarking – HySEA experiments (2017)

- Once again, there are discrepancies and scatter among the predictions, which highlights the need for better guidance
- It is noted that the engineering models generally performed better than the more advanced CFD-based consequence models.



Skjold, et al, 2017

Validation and consistency across industry

Need for development of good practice guidance

- This isn't just a concern for modelling hydrogen explosions – there is a clear need for better guidance across many applications
- Whilst for many applications there may be high-level agreement on a particular approach, the **devil is in the detail**, and without better practical guidance individual practitioners necessarily develop their own bespoke methods which inevitably leads to **inconsistencies in simulation approach**
- This is damaging to the credibility of the CFD approach.

Validation and consistency across industry

Steps forward – NAFEMS

- NAFEMS (http://www.nafems.org/) is the international association for the engineering simulation community
- NAFEMS focusses on the practical application of numerical engineering simulation techniques including finite element analysis, computational fluid dynamics, and multibody simulation
- NAFEMS has established a focus group to develop good practice guidance for selected CFD applications in the oil and gas sector:
  - review existing guidance relating to the use of CFD for selected routine applications, and identify where there are gaps within the existing guidance
  - develop a coordinated series of *How To* guides to provide practical guidance for simulation users in the industry.

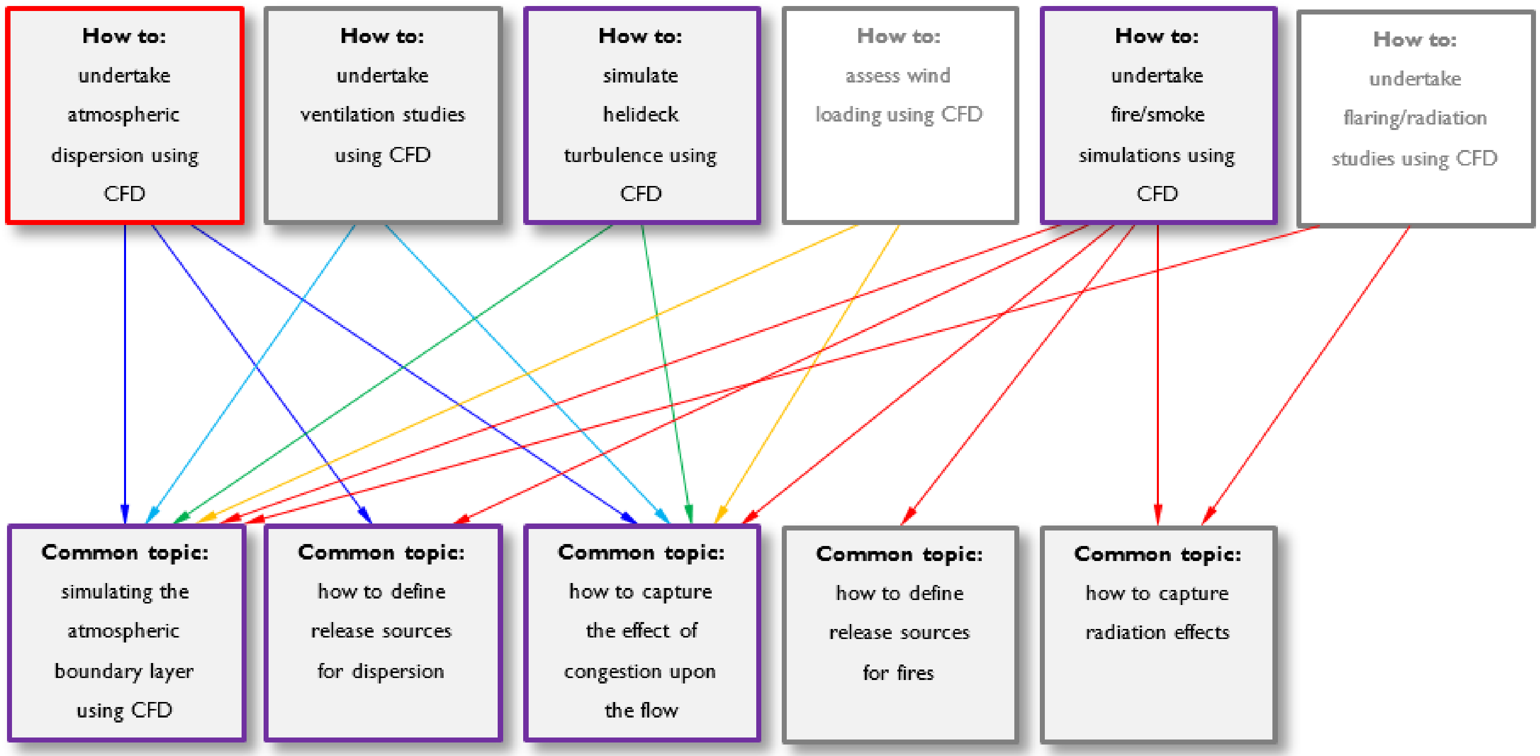
Validation and consistency across industry

What will be included in terms of guidance?

- High-level guidance for simulation engineers and the wider team:
  - discussion of the wider physics that should be considered
  - flowcharts to advise on which simulation approach is fit for purpose
  - checklists/templates/workflows to ensure that all of the important physics are captured
- Detailed guidance specifically for hands-on simulation engineers:
  - worked examples with real numbers relating to the underlying physics that can usefully be used for the purpose of CFD verification
- Blind benchmarking tests to identify inconsistencies in approach
- Identification of potential shortcomings of CFD software.

Validation and consistency across industry

Proposed document structure for technical safety

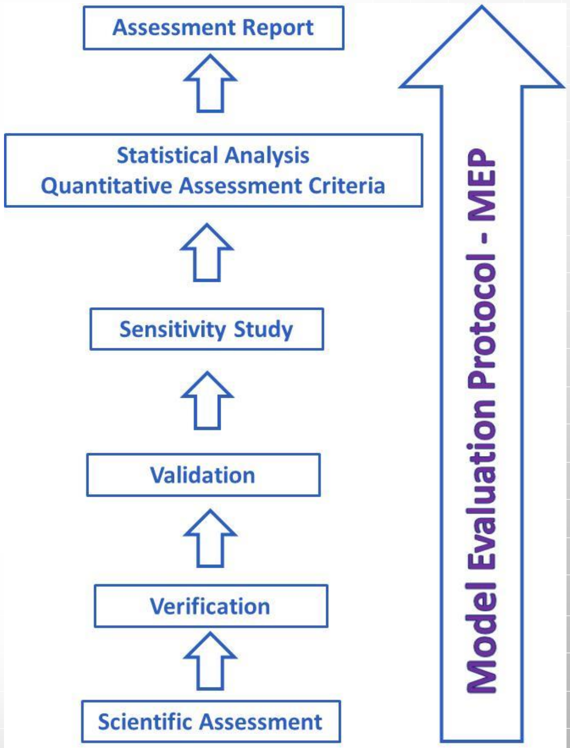


SUSANA project

- SUpport to SAfety ANalysis of Hydrogen and Fuel Cell Technologies (www.support-cfd.eu)
- The SUSANA project (co-funded by the Fuel Cell and Hydrogen Joint Undertaking): producing a Model Evaluation Protocol for hydrogen technologies safety (HyMEP)

SUSANA project

- HyMEP:
  - The first MEP for hydrogen technologies safety
  - To evaluate the accuracy of the CFD models
  - To assess user capability of correctly using CFD codes
- Current version of database (www.support-cfd.eu) including ~30 experiments
- Current Status:
  - Limited benchmarking and progress made as a part of the SUSANA project to resolve differences seen (special edition of FABIG meeting)
  - Not a very large participation
  - Significant work remains to be done



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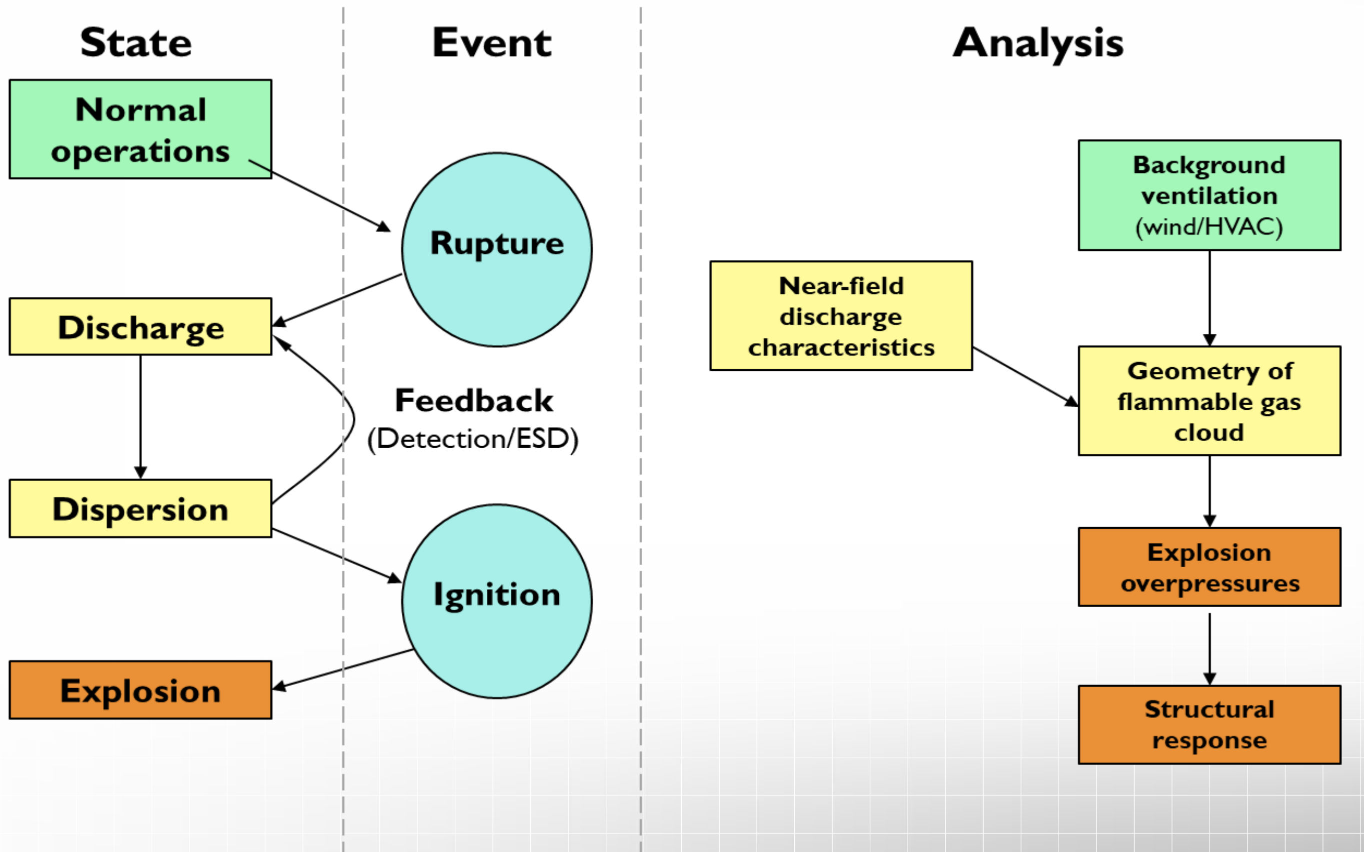
Explosion risk analysis

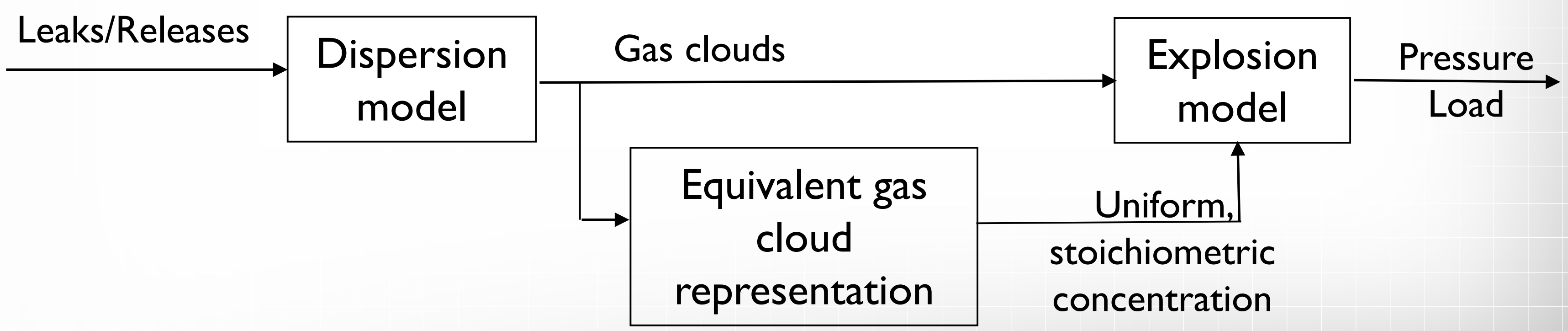
Explosion modelling – integrated approach



Explosion risk analysis

Equivalent gas cloud methods

- One of the major challenges for CFD-based probabilistic QRA is limiting the total number of scenarios to simulate
- A key consideration is which *equivalent gas cloud* method to use to couple the dispersion and explosion phases of the study.



Explosion risk analysis

Equivalent gas cloud methods

- There are 4 equivalent gas cloud methods that can be envisioned:
  - direct mapping of inhomogeneous clouds
  - any region above the LFL is assumed to be stoichiometric
  - any region between the LFL and UFL is assumed to be stoichiometric
  - the equivalent stoichiometric volume approach (Q8 or Q9)

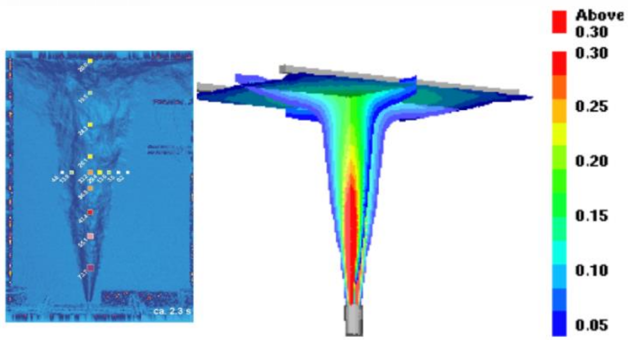
$$Q9 = \sum(\text{vol} \times S \times E) / (S \times E)_{max}$$
$$Q8 = \sum(\text{vol} \times E) / (E)_{max}$$

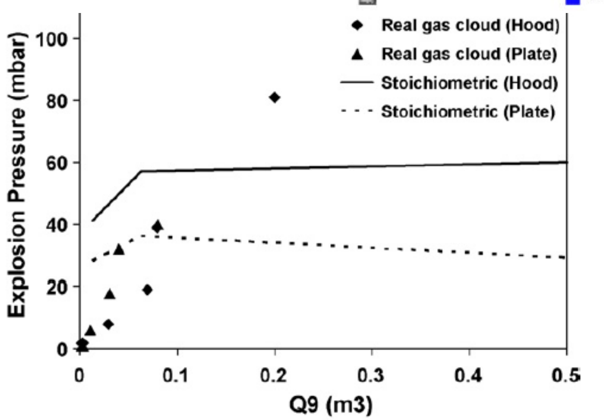
- Validation is required to identify the preferred approach for hydrogen – controlled release and ignition tests.

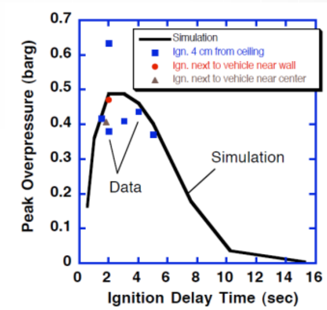
Explosion risk analysis

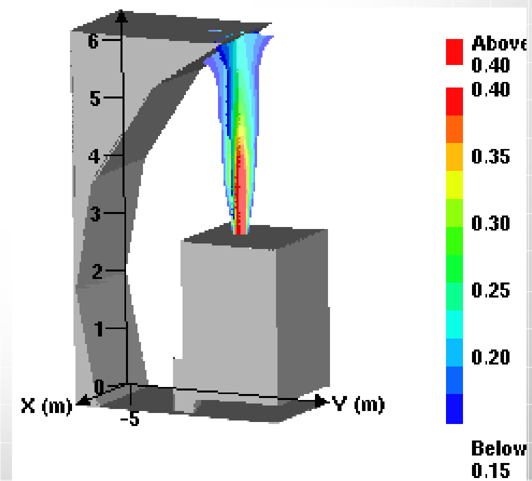
Equivalent gas cloud methods

Validation against experiments – FZK/KIT and Sandia









Explosion risk analysis

Equivalent gas cloud methods – observations

- For a confined scenario, or a scenario where very high flame speeds are expected, use a weighting of reactivity, Q8
- For unconfined situations one could reduce the conservatism and use a weighting of reactivity and expansion, Q9
- Although Q9 method gives a reasonable description of expected severity, there remain some uncertainties:
  - effect of jet-induced turbulence (can increase overpressure 2-3 times)
  - rich clouds (and stratified layers) may get diluted to stoichiometric when flame pushes unburnt fuel inside rooms or outside vent openings
- Q8/Q9 methods may be better for hydrogen?

Explosion risk analysis

Equivalent gas cloud methods – observations (location/shape)

- Buoyancy is strong – assume any confined/semi-confined cloud is located below the ceiling or other horizontal confinement
- For a low momentum release in a confined situation with strong stratification, the cloud should be assumed to cover full ceiling area (or area between structural beams)
- For a free jet in a less confined situation:
  - jet momentum will usually dominate the mixing of the jet until the hydrogen concentration has become lean
  - the cloud should be assumed to be located a small distance downwind
  - the aspect ratio for a free cloud should be 1:1:1, for a cloud towards the ceiling 2:2:1, towards ceiling with one sidewall 2:1:1.

Agenda

- Background and introduction
- Modelling and simulation
- CFD analysis
- Validation and consistency across industry
- Explosion risk analysis
- Probabilistic structural response
- Summary

Probabilistic structural response

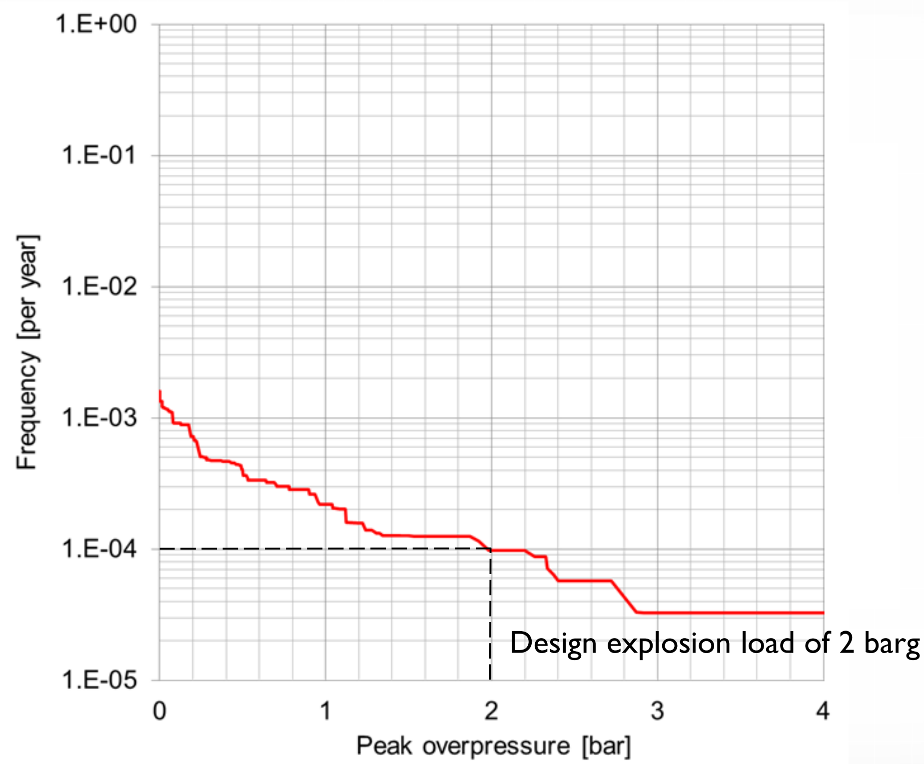
Mitigation

- Hydrogen explosions can be catastrophic – it is therefore imperative to have appropriate mitigation measures in place, which may include, for example, venting, inerting, and the use of water mist
- The use of *protection walls* is seemingly easiest, although their design can be prohibitive due to highly localised explosion loads
- It is, therefore, important to account for these localised effects by using methods such as the 3D risk approach and one-to-one CFD/FEA coupling, in order to reduce conservatism in the design
  - these approaches are demonstrated for a blast wall with conventional fuel (from our recent FABIG paper http://abercus.com/News_20161130.aspx).

Probabilistic structural response

3D risk assessment (conventional fuel)

For this exceedence curve, the 10^{-4}/yr peak overpressure for the blast wall is 2 barg



Probabilistic structural response

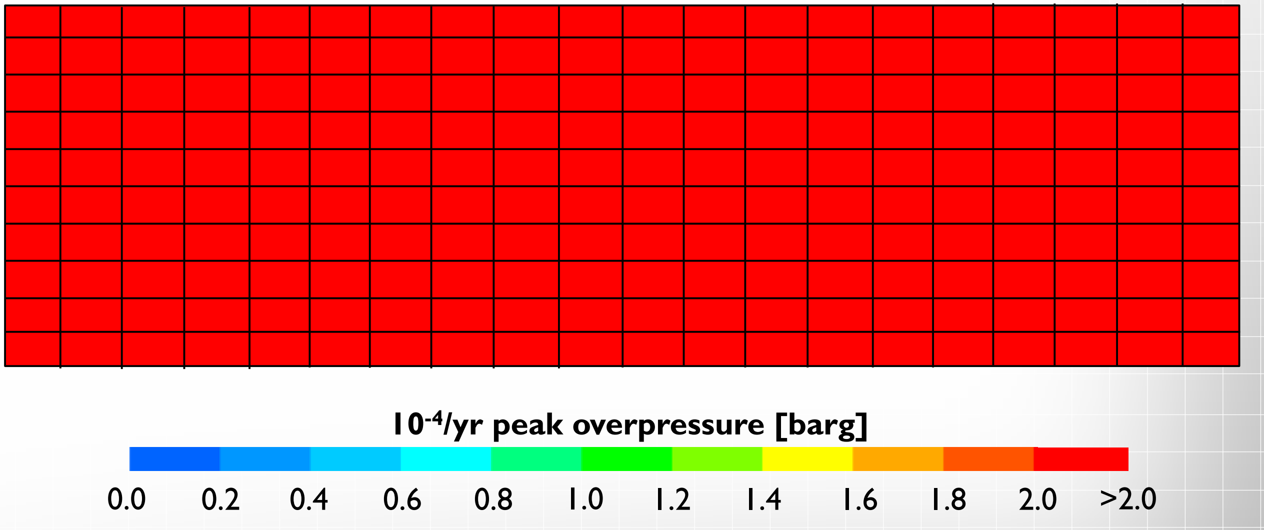
3D risk assessment (conventional fuel)

For this exceedence curve, the 10^{-4}/yr peak overpressure for the blast wall is 2 barg

Typically this would be applied uniformly across a large object, such as a blast wall.

Contours of 10^{-4}/yr peak overpressure

Large objects are typically represented by a discretised array of monitor panels within the CFD model



Probabilistic structural response

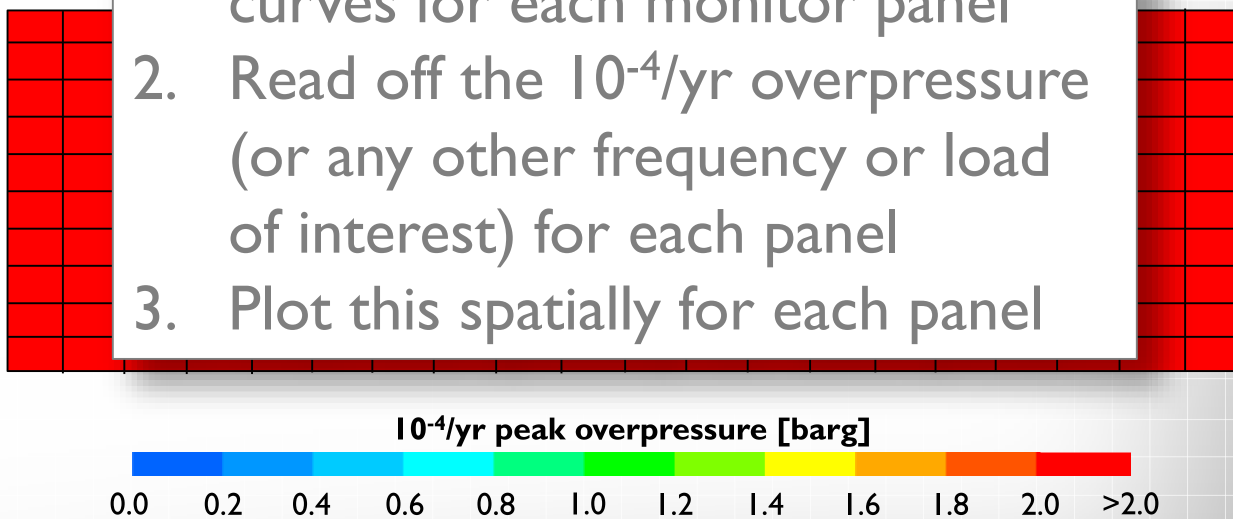
3D risk assessment (conventional fuel)

For this exceedence curve, the 10^{-4}/yr peak overpressure for the blast wall is 2 barg

Typically this would be applied uniformly across a large object, such as a blast wall.

Contours of 10^{-4}/yr peak overpressure

1. Compile separate exceedance curves for each monitor panel
2. Read off the 10^{-4}/yr overpressure (or any other frequency or load of interest) for each panel
3. Plot this spatially for each panel

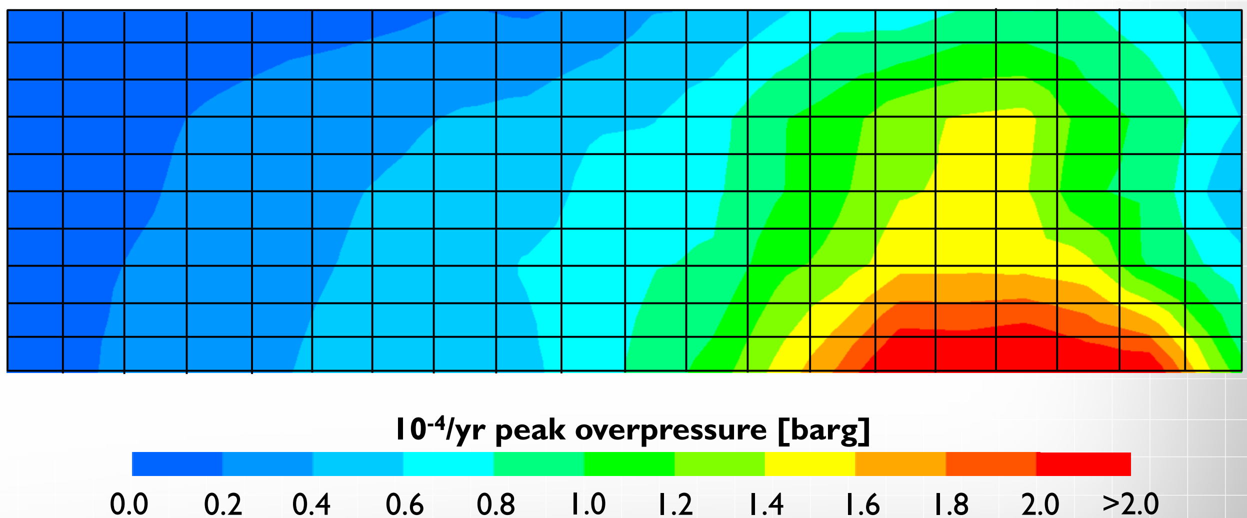


Probabilistic structural response

3D risk assessment (conventional fuel)

If exceedence curves are constructed separately for each panel, the spatial variation of the 10^{-4}/yr peak overpressure can be considered.

Contours of 10^{-4}/yr peak overpressure



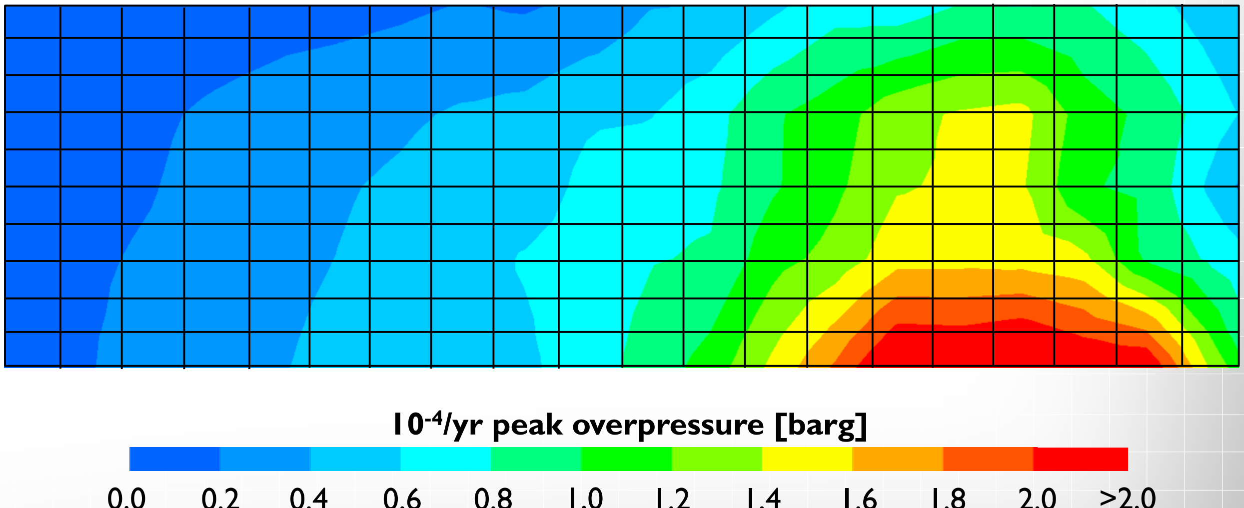
Probabilistic structural response

3D risk assessment (conventional fuel)

The 10^{-4}/yr peak overpressure for the majority of the blast wall is significantly less than 2 barg in this example

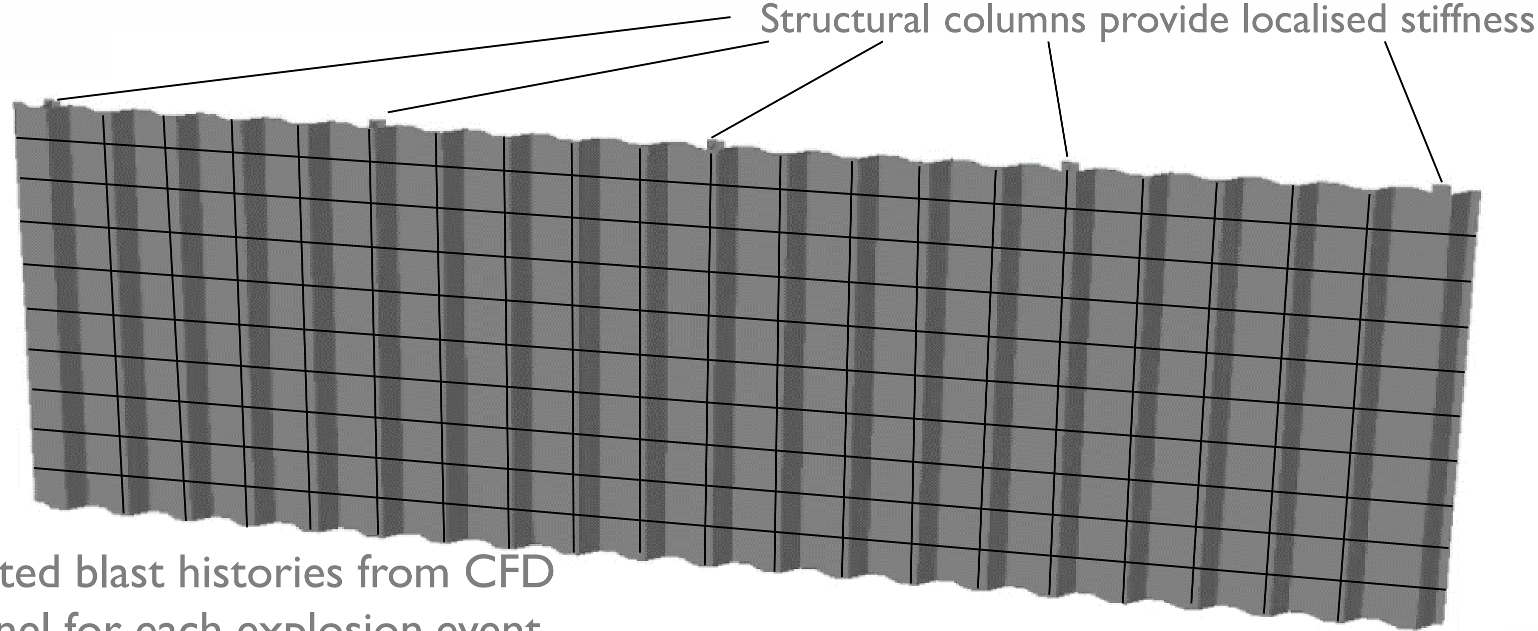
This can have a significant impact upon the structural response of the blast wall under DAL loading.

Contours of 10^{-4}/yr peak overpressure



Probabilistic structural response

One-to-one CFD/NLFEA coupling (conventional fuel)

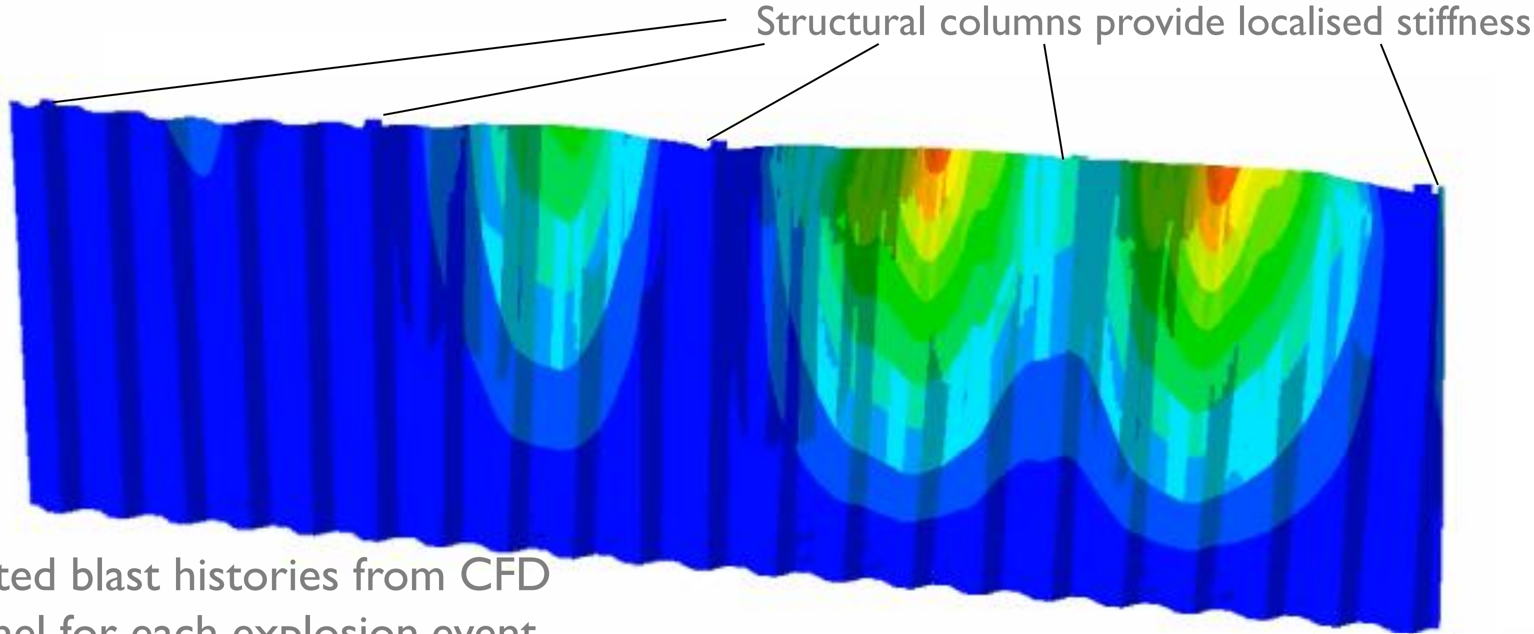


Map predicted blast histories from CFD at each panel for each explosion event

Structure of the blast wall

Probabilistic structural response

One-to-one CFD/NLFEA coupling (conventional fuel)

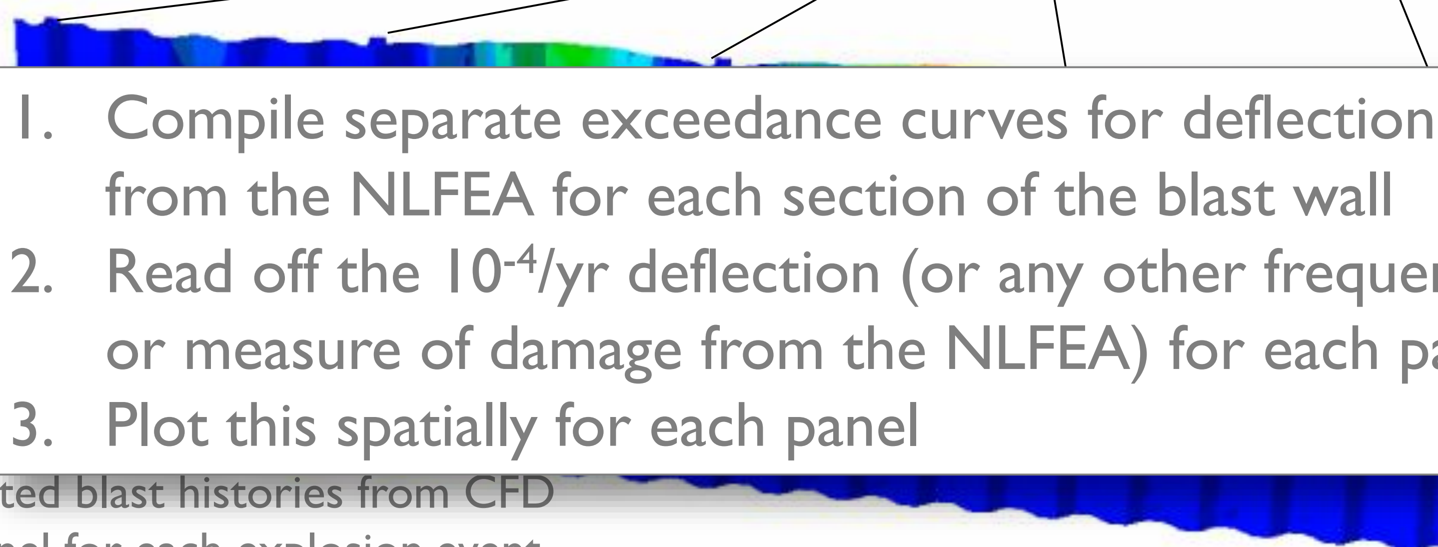


Map predicted blast histories from CFD at each panel for each explosion event

Structure of the blast wall

Probabilistic structural response

One-to-one CFD/NLFEA coupling (conventional fuel)



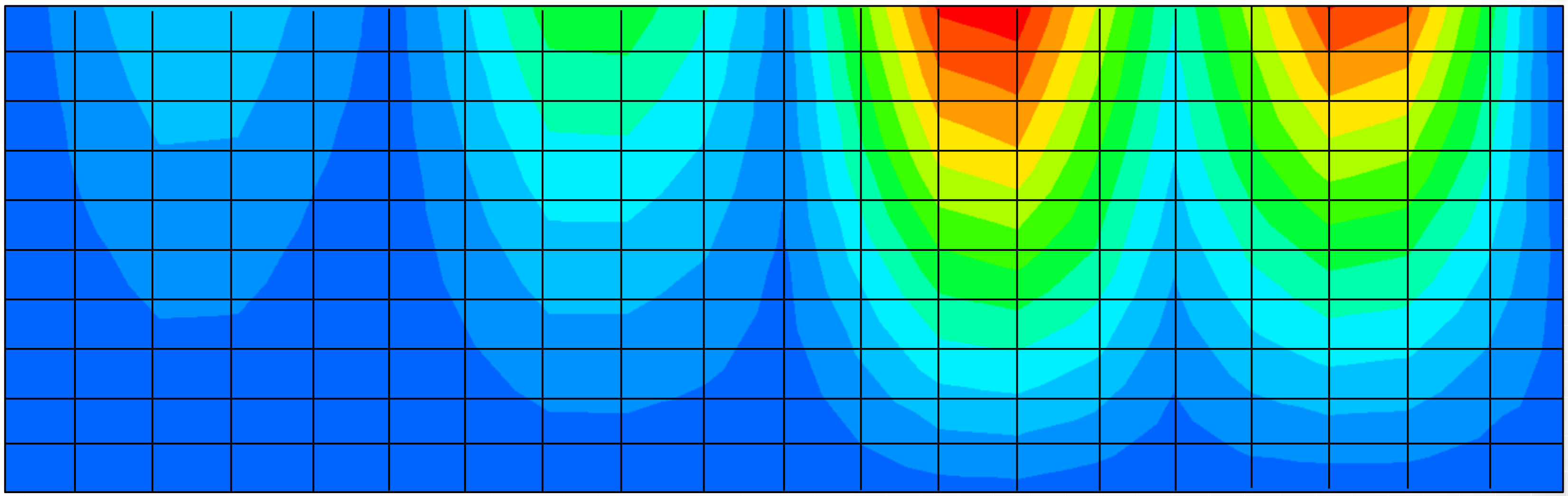
1. Compile separate exceedance curves for deflection from the NLFEA for each section of the blast wall
2. Read off the 10^{-4}/yr deflection (or any other frequency or measure of damage from the NLFEA) for each panel
3. Plot this spatially for each panel

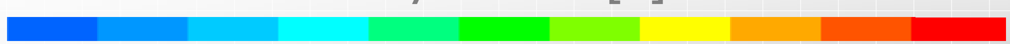
Structure of the blast wall

Probabilistic structural response

One-to-one CFD/NLFEA coupling (conventional fuel)

Contours of 10^{-4}/yr deflection

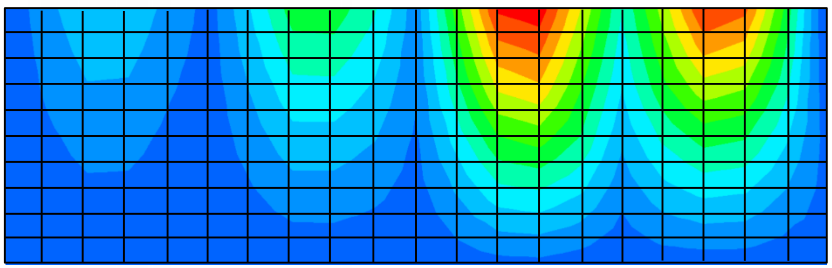




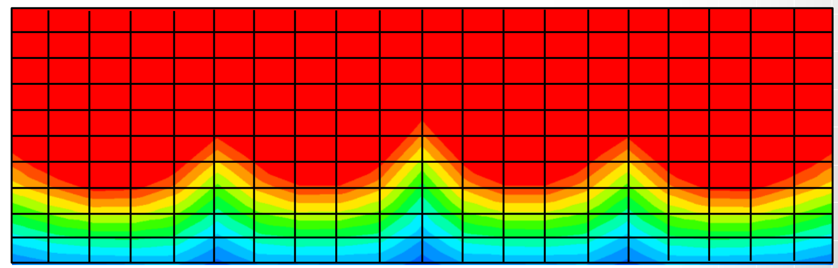
Probabilistic structural response

One-to-one CFD/NLFEA coupling (conventional fuel)

Contours of 10^{-4}/yr deflection

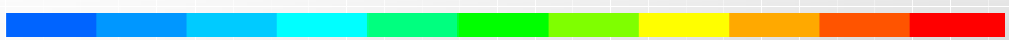


Using one-to-one CFD/NLFEA coupling



Traditional approach – uniformly applying the 10^{-4}/yr overpressure (2 barg) from the exceedance curve

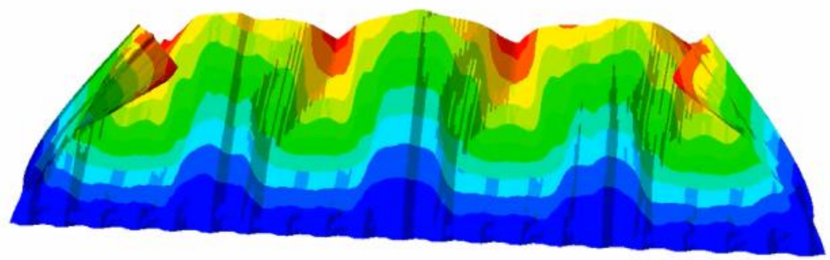
10^{-4}/yr deflection [m]



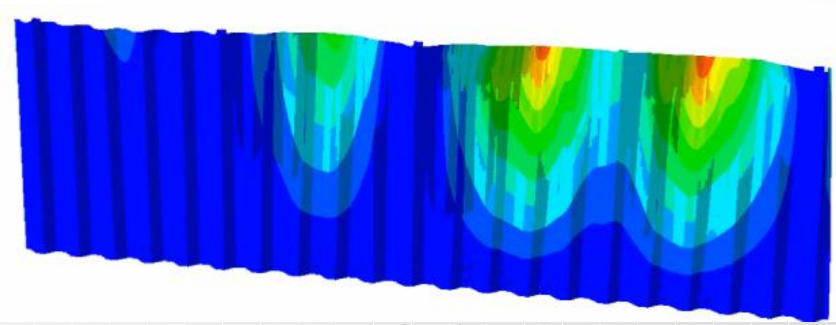
Probabilistic structural response

One-to-one CFD/NLFEA coupling (conventional fuel)

It is clear is that the traditional approach with a uniformly applied 10^{-4}/yr load is overly conservative when compared to the one-to-one CFD/NLFEA coupling approach.



Traditional approach – uniformly applying the 10^{-4}/yr overpressure (2 barg) from the exceedance curve



Using one-to-one CFD/NLFEA coupling

Probabilistic structural response

CFD/NLFEA coupling (hydrogen explosions)

HySEA project (Skjold, et al, 2017)

STRUCTURAL RESPONSE FOR VENTED HYDROGEN DEFLAGRATIONS: COUPLING CFD AND FE TOOLS

Atanga, G.[1], Lakshmipathy, S.[1], Skjold, T.[1], Hisken, H.[1] and Hanssen, A.G.[2]

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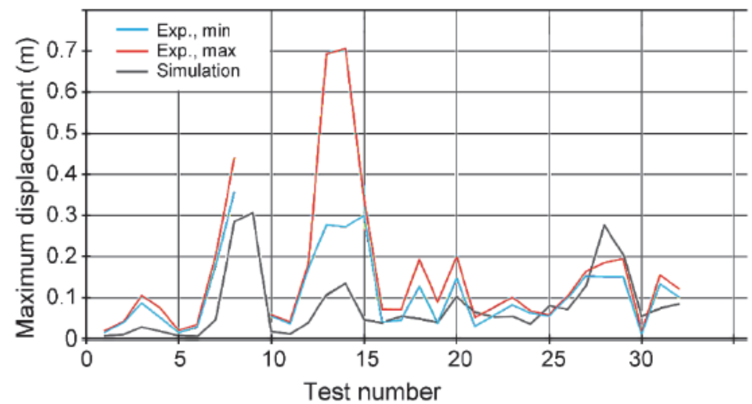

Full spatial mapping of explosion loads predicted with the CFD (FLACS) to NLFEA (IMPETUS Afea)

Maximum displacement of sidewalls for 34 tests

Agenda

Background and introduction

Modelling and simulation

Application of computational fluid dynamics

Validation and consistency across industry

Explosion risk analysis

Probabilistic structural response

Summary

Summary

- Hydrogen is quite different from conventional fuels
  - buoyancy will quickly remove accumulated hydrogen when unconfined
  - the flammable range is wider (although the LFL is not so different)
  - hydrogen is more reactive
  - a hydrogen deflagration is more likely to transition to detonation
  - lower energies are needed to ignite hydrogen
  - the J-T coefficient for hydrogen is negative, so a leaking gas *warms*, which increases the likelihood of spontaneous ignition.

Summary

- CFD modelling is an appropriate tool to understand the consequences of hydrogen explosions, including DDT, but the reliability/accuracy of CFD remains a significant concern
- There is a need for consistent validation efforts within industry
  - even if there is high-level agreement on a particular approach, the devil is in the detail
  - without better practical guidance individual practitioners necessarily develop their own bespoke methods which inevitably leads to inconsistencies in simulation approach
  - blind benchmarking exercises can help to demonstrate this
  - there is a need for development of practical good practice guidance
  - organisations such as NAFEMS can play a role.

Summary

- Specific considerations for carrying out a probabilistic explosion analysis
  - effect of buoyancy on gas cloud – horizontal obstructions
  - use of equivalent stoichiometric gas cloud
  - shall we account for stratification in the cloud?
- Hydrogen explosions can lead to highly localised explosion loads
  - these localised effects can be accounted for by using methods such as the 3D risk approach and one-to-one CFD/FEA coupling
  - these approaches can help to reduce conservatism in design of mitigation measures such as protection walls.

Contact us

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