MODELLING EXPLOSIONS IN REALISTIC GEOMETRY WITH PDRFOAM

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Pratap Sathiah, Jonathan Puttock, Debapriya Chakraborty and Walter Farmayan

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Resources: Our use of the term "resources" in this presentation includes quantities of oil and gas not yet classified as SEC proved oil and gas reserves. Resources are consistent with the Society of Petroleum Engineers 2P and 2C definitions.

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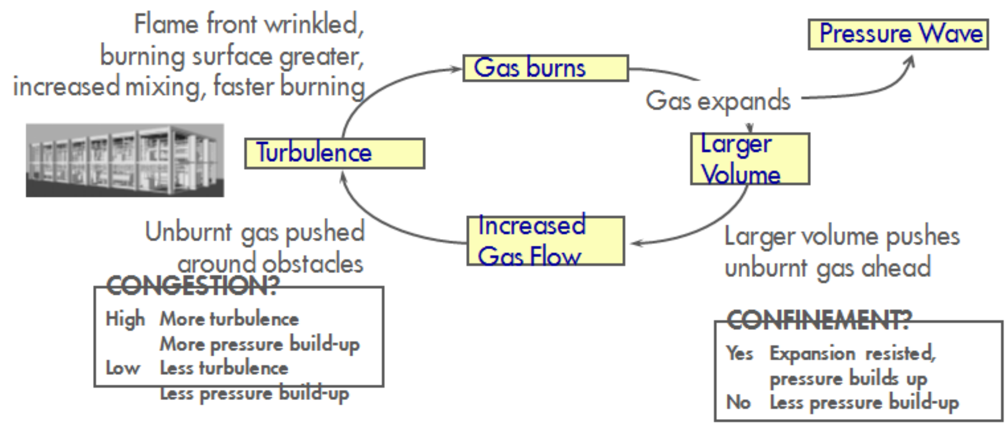
AGENDA

- Schelkin Mechanism.
- Porosity Distributed Resistance Approach (PDR).
- PDR field generation and combustion model in PDRFoam
- Validation of PDRFoam
- Conclusion
- Future work

MODELLING CONGESTED VAPOUR CLOUD EXPLOSIONS

Schelkin Mechanism:

- When the unburnt gas mixture comes in contact with obstacle it generates turbulence.
- Turbulence generation increases the flame wrinkling, thereby increasing the overpressure.



Schelkin Mechanism

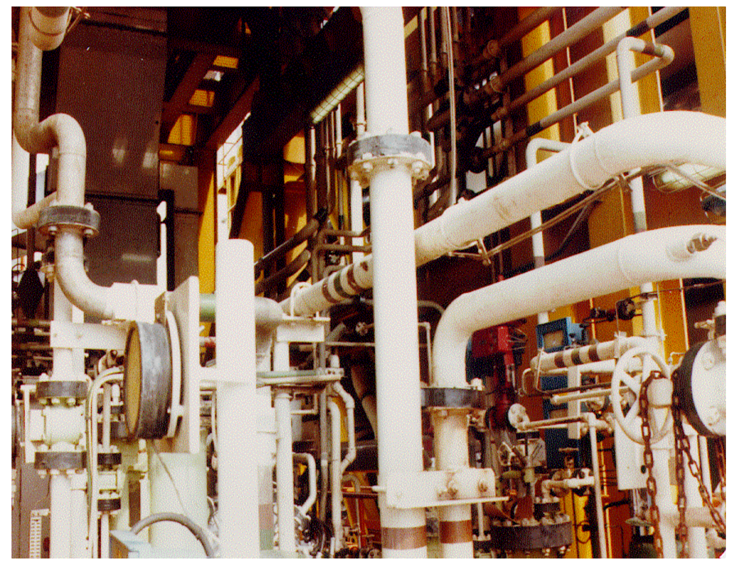
Modelling methods:

- Empirical approaches e.g. CAM, MEM and TNO
- Phenomenological approaches e.g. SCOPE and CLICHE
- CFD based approaches e.g. FLUENT, CFX and STAR CCM+

PROBLEM WITH CFD BASED APPROACHES

Real plant is complex (very)...

■ Real Plant



■ Zoom out

THE RESOLUTION PROBLEM

- The CAD representation of a petrochemical unit may contain hundreds of thousands or even millions objects.
- Pipes down to dimensions of 50mm or less can have a significant effect on the flame surface area, hence the rate of combustion, hence explosion development.
- Using a million computational cells, we can typically use a cell size of about 0.5 m.
- Fully-resolved computations would requires 100 million mesh domain. So would perhaps need computers with a million times greater capacity.

Hence the use of sub-grid modelling – "Porosity Distributed Resistance (PDR) Approach".

POROSITY/DISTRIBUTED RESISTANCE (PDR) APPROACH

It is an approach were small scales associated with small obstacles are modelled while large scales associated with large obstacles are resolved. This essentially means that drag, turbulence and flame enhancement due to the small obstacles are represented as source and sink term in the respective equations.

This approach is commonly used in other vapor cloud explosion codes FLACS, EXSIM and COBRA. PDRFoam is also based on this concept.

SUB-GRID TERMS IN , E.G. CONTINUITY, MOMENTUM AND TURBULENCE EQUATIONS

Continuity:

$$\frac{\partial}{\partial t}[\beta_v \rho] + \frac{\partial}{\partial x_i}[\beta_i \rho u_i] = 0$$

Momentum:

$$\frac{\partial}{\partial t}[\beta_v \rho u_i] + \frac{\partial}{\partial x_j}[\beta_j \rho u_j u_i] + \beta_v \frac{\partial p}{\partial x_i} - \beta_v \rho g_i = \frac{\partial}{\partial x_j}[\beta_j \sigma_{ij}] + R_i$$

Turbulence:

$$\frac{\partial}{\partial t}[\beta_v \rho k] + \frac{\partial}{\partial x_j}[\beta_j \rho u_j k] = \frac{\partial}{\partial x_j}\left[\beta_j \frac{\mu_{eff}}{\sigma_k}\frac{\partial k}{\partial x_j}\right] + G - \beta_v \rho \varepsilon$$

$$\frac{\partial}{\partial t}[\beta_v \rho \varepsilon] + \frac{\partial}{\partial x_j}[\beta_j \rho u_j \varepsilon] = \frac{\partial}{\partial x_j}\left[\beta_j \frac{\mu_{eff}}{\sigma_k}\frac{\partial \varepsilon}{\partial x_j}\right] + C_1 \frac{\varepsilon}{k} G - C_2 \beta_v \rho \frac{\varepsilon^2}{k}$$

$$G = G_r + G_s$$

R_i : Resistance due to sub-grid obstacles

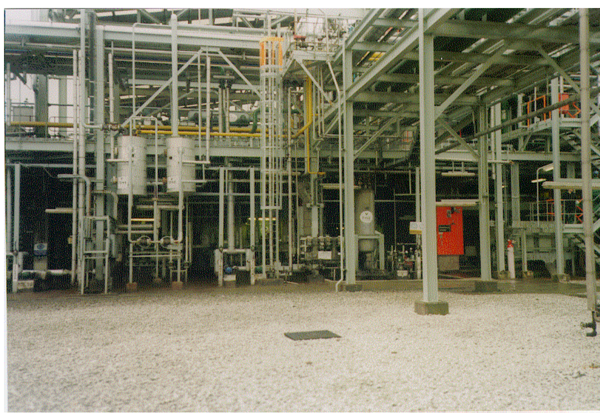
β_i : Area porosity β_v : Volume porosity

G_r: Turbulent kinetic production due to unresolved obstacles

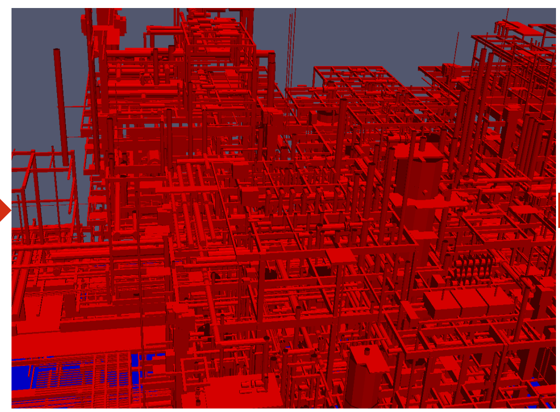
POROSITY/DISTRIBUTED RESISTANCE APPROACH

- Convert geometry to cell-wise values of:
  - Porosity (area and volume)
  - (Tensor) drag
  - Turbulence generation

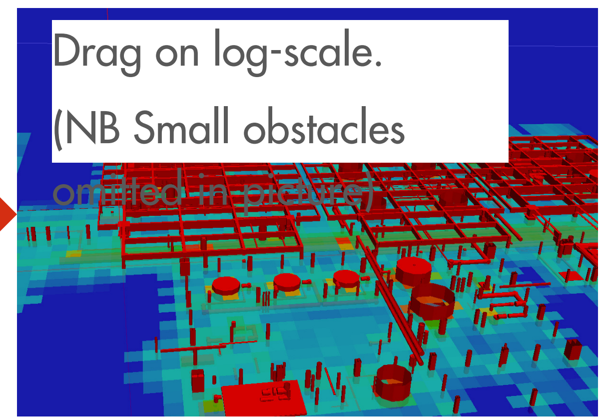
CAD_PDR (Shell's Internal Tool)



- Real plant



- CAD File



- PDR Representation

CAD_PDR- SHELL'S TOOL FOR GENERATING PDR FIELDS (1)

- CAD_PDR takes lists of obstacles (derived from CAD) as input, e.g.:
  - Cuboid or flat plane – may be porous
  - Diagonal beam
  - Cylinder, aligned with principal axes
  - Blow-off panel
  - Patch, where a specific boundary condition can be applied

CAD_PDR- SHELL'S TOOL FOR GENERATING PDR FIELDS (2)

- CAD_PDR calculates fields required by the PDR CFD model cell by cell on the mesh. For example:
  - Area porosities in the mass and diffusion fluxes
  - Volume porosities in appropriate source and transient terms
  - Sub-grid obstacle resistance (drag tensor)source term in momentum equations
  - Sub-grid obstacle turbulence source term in k-epsilon equations (with length scale related to obstacle diameter)
  - Sub-grid flame area source term enhances combustion (in addition to effect of turbulence increase).

COMBUSTION MODEL

- The combustion model (same as available in OpenFoam package XiFoam) solves a progress variable equation.
- The source term is closed using turbulent flame speed which is obtained by solving equations for the flame wrinkling factor.
- For the quasi-laminar flame propagation phase a simple model is used.
- Effects of compression is taken into account in laminar flame speed, unburnt gas density and unburnt thermal diffusivity.

$$\bar{\rho}\frac{\partial \tilde{c}}{\partial t} + \bar{\rho}\tilde{u}_k \frac{\partial \tilde{c}}{\partial x_k} = \frac{\partial}{\partial x_k}\left(\bar{\rho} D_t \frac{\partial \tilde{c}}{\partial x_k}\right) + \rho_u U_t \left|\nabla \tilde{c}\right|$$

Ξ: the ratio of the average flame surface area to the average flame area projected in the direction of mean flame propagation. This is the same as the local ratio of the turbulent and laminar flame speeds.

$$U_{t,\ quasi} = Sl + aR;$$

R: is the flame radius

$$S_l = S_{l,0}\left(\frac{p}{p_0}\right)^m \left(\frac{T}{T_0}\right)^n = S_{l,0}\left(\frac{p}{p_0}\right)^\alpha$$

$$\rho_u = \rho_{u,0}\left(\frac{p}{p_0}\right)^{1/\gamma},$$

$$\kappa_u = \kappa_{u,0}\left(\frac{T}{T_0}\right)^a \left(\frac{p}{p_0}\right)^b$$

SUBMODEL FOR FLAME WRINKLING FACTOR Ξ

Flame wrinkling factor Ξ is divided into contribution from turbulence Ξ_T and from sub grid objects Ξ_S.

This means that turbulent flame speed is calculated as follows:

$U_t = \Xi_T \, \Xi_S \, S_l$.

A correlation for turbulent burning velocity based on recent data [Bradley et al. 2013], allowing for positive and negative Markstein numbers, and quench at high Karlowitz number is used to calculate flame wrinkling contribution from turbulence Ξ_T.

STEPS IN EXPLOSION MODELLING USING CAD_PDR/PDRFOAM

Steps

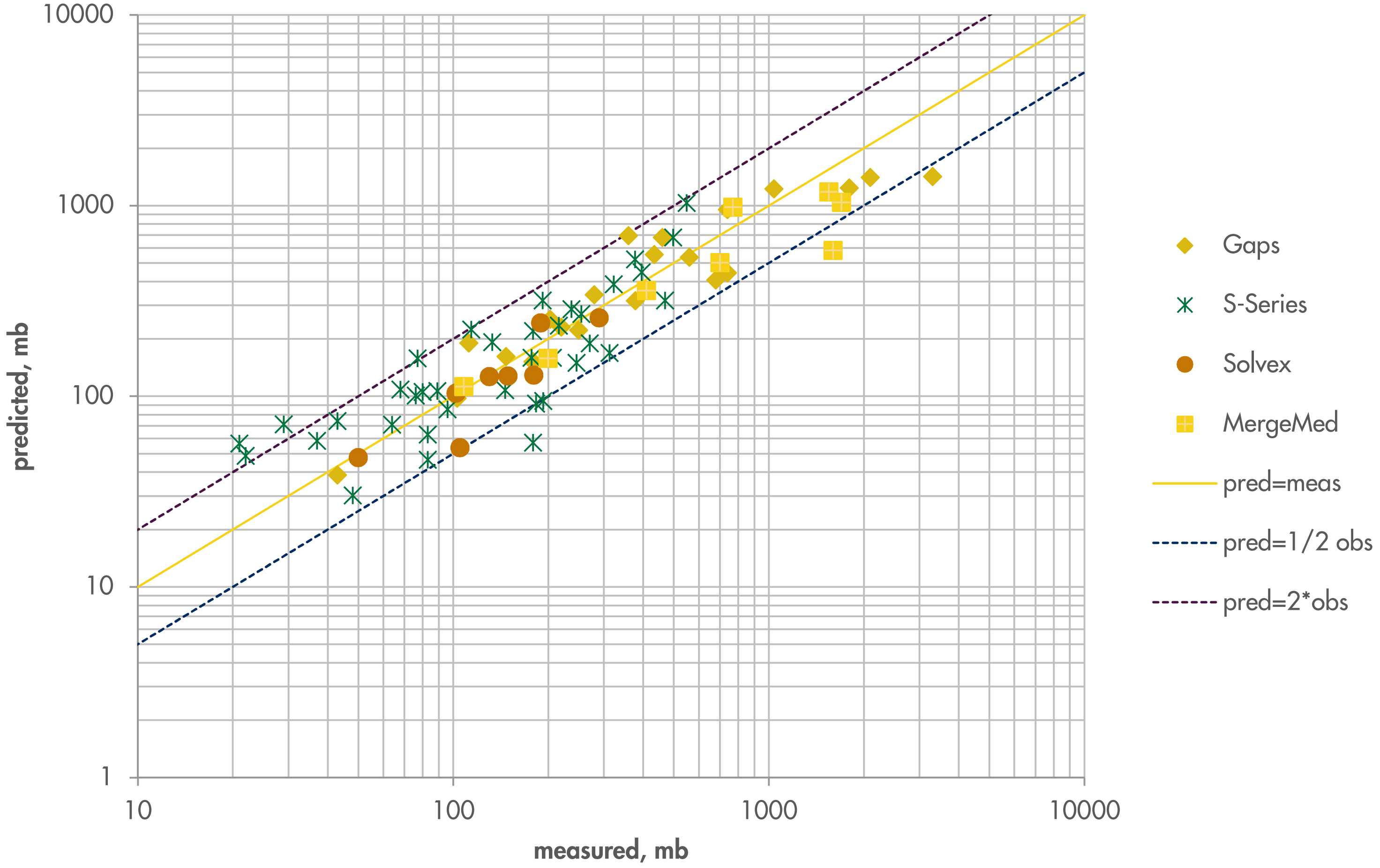
- Mesh planes automatically fitted to large obstacles and surfaces (PDRFitMesh)
- Program (CAD_PDR) to read CAD files (up to and derive sub-grid parameters per computational cell
- Blocked cells removed from mesh (PDRMesh)
- Internal surfaces (baffles)
- CFD run (PDRFoam)

EXPERIMENTAL VALIDATION– SMALL SCALE

- Validation test matrix

Case	Fuels
Gaps	Propane, Methane and Ethene
Solvex	Propane and Methane
Merge Medium	Propane, Methane and Ethene
Buxton S Series	Propane, Methane, Ethene and Hydrogen
Gaps(Ergos)	Propane, Methane, Ethene and Hydrogen

RESULTS - SMALL SCALE VALIDATION – OVERPRESSURE

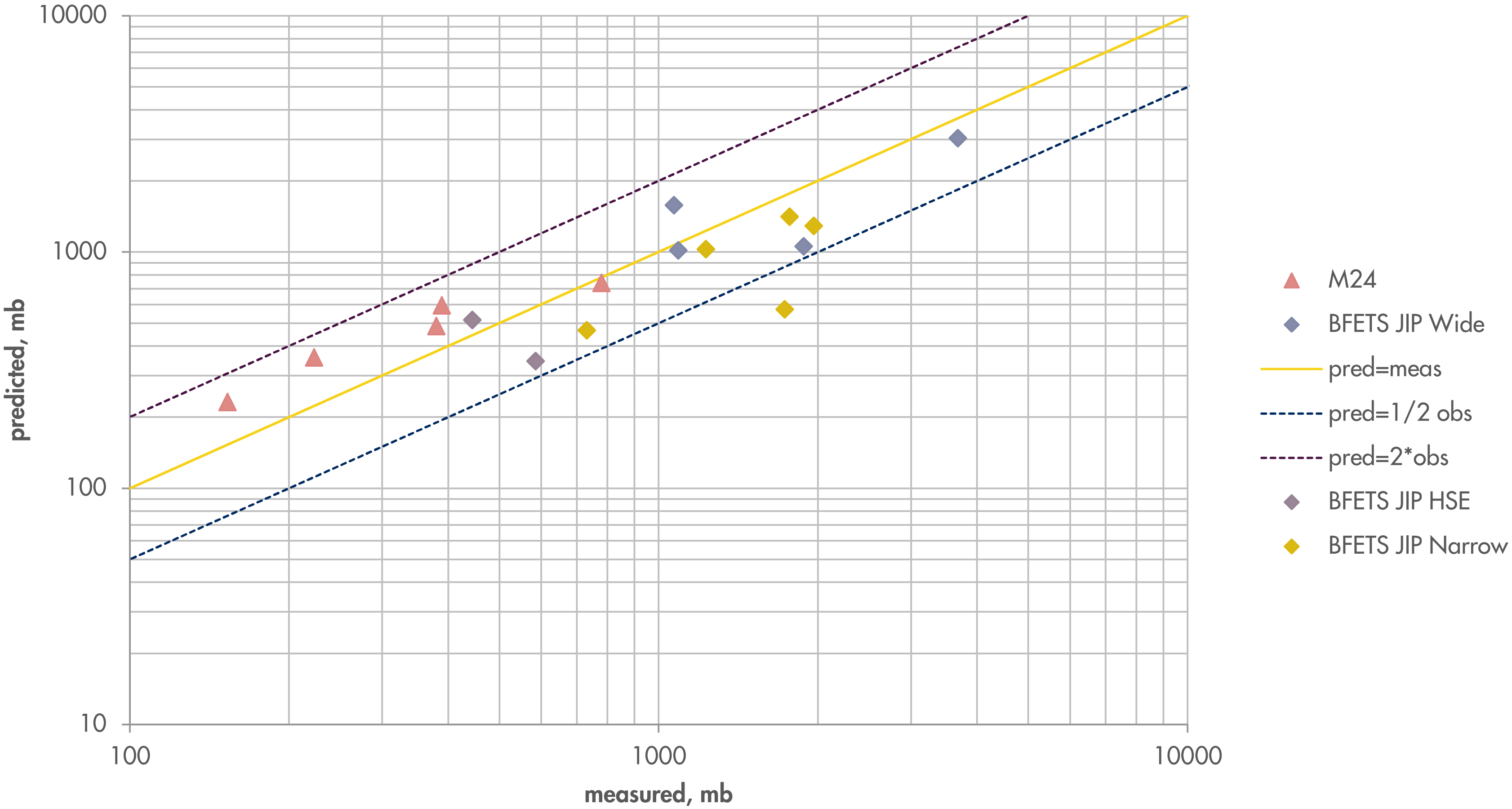


EXPERIMENTAL VALIDATION – LARGE SCALE

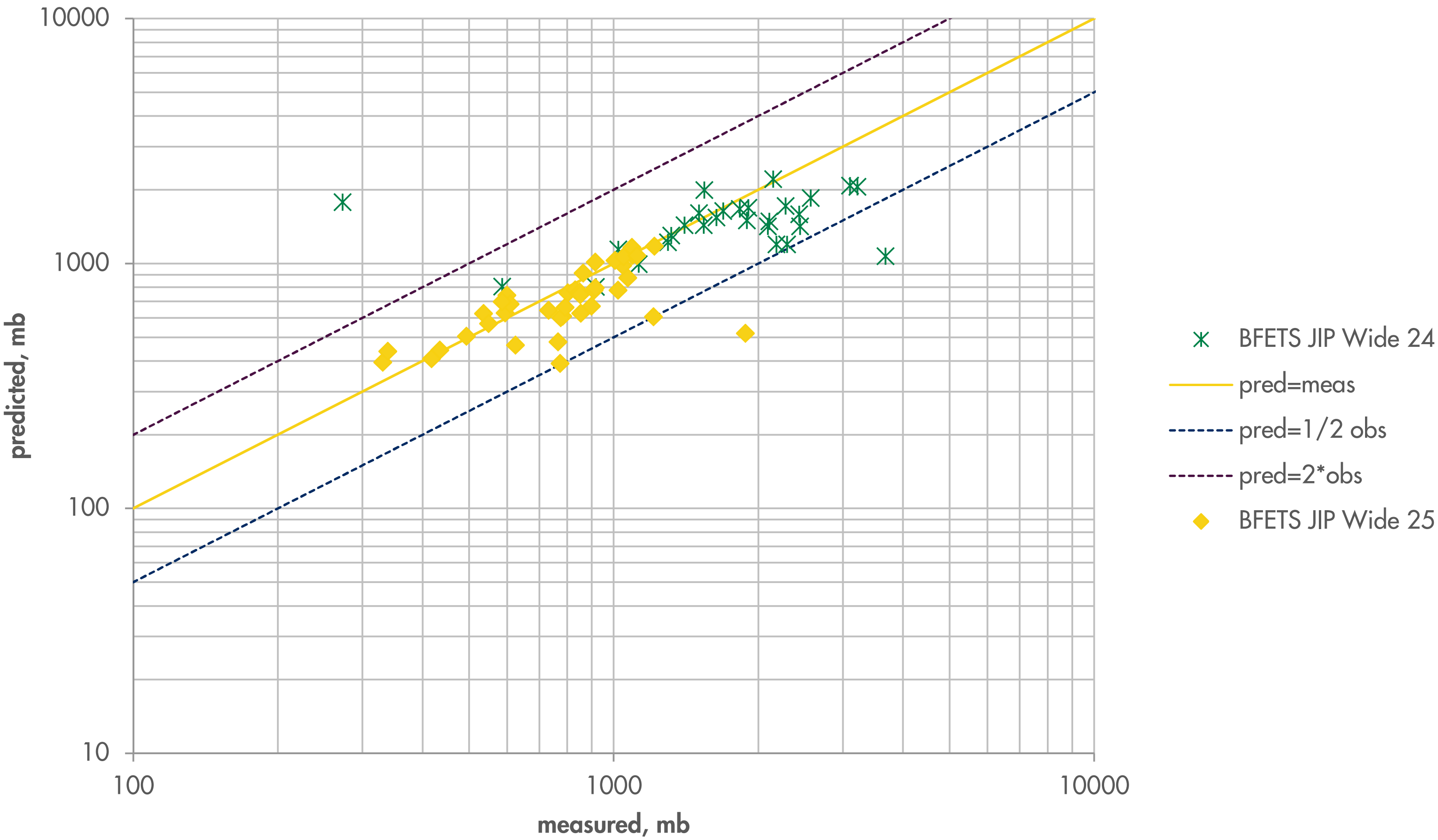
- Validation test matrix

Case	Fuel
CMI M24	Propane and Methane
BFETS Phase 2 JIP Narrow	Methane
BFETS Phase 2 JIP Wide	Methane
BFETS Phase 3 HSE	Methane

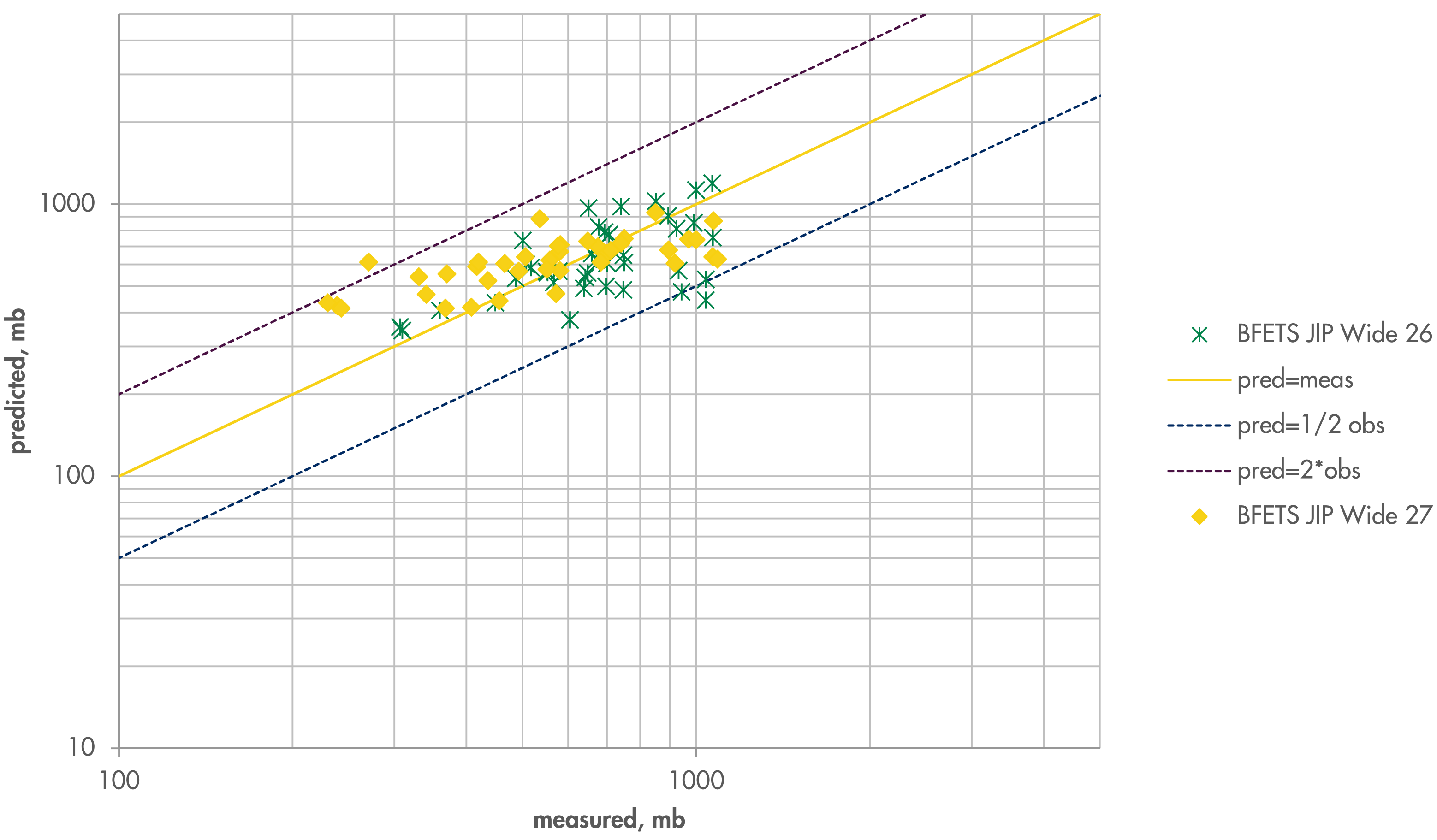
RESULTS - LARGE SCALE VALIDATION – MEDIAN OVERPRESSURE



RESULTS - LARGE SCALE VALIDATION – OVERPRESSURE (1)



RESULTS - LARGE SCALE VALIDATION – OVERPRESSURE (2)



CONCLUSIONS

CAD_PDR/PDRFoam has the following features:

- Input from obstacle files, derived from CAD, with a range of obstacle types, including diagonal beams, allowing for intersecting obstacles.
- Use of the Weller's combustion model and correlation for turbulent burning velocity based on recent data, allowing for positive and negative Markstein numbers, and quench at high Karlowitz number.
- Validation results against small scale and large scale experiments were performed using PDRFoam. Maximum overpressure, median of overpressure and maximum overpressure at each probe points are predicted within the accuracy of ± 50 % for four different fuels.

OTHER FUNCTIONALITIES

- Efficient parallelization of the code
- Non-orthogonal external mesh extending to infinity.
- Auto fitting mesh planes to obstacle faces, fitting of the mesh to large obstacles and to distant buildings.
- Adaptive mesh refinement (AMR) to capture flame propagation and pressure wave needed to accurately predict pressure decay.
- Flame quenching, advection of flame area and persistence of flame area generation outside congestion.
- Option to use different turbulence models for explosion analysis.

FUTURE WORK

- Further validations against small scale experiments e.g. Solvex 1/6, quarter box and large scale experiments (BFETS Phase 2 and Phase 3).
- Extension of the model for non-uniform gas clouds / fuel-air mixtures and subsequent validations against large scale BFETS Phase 3B experiments.
- Validation of the model for explosion mitigations i.e. to the cases where water deluge was used to mitigate explosion.
- Working on criteria to predict deflagration to detonation transition.
- Combine with OpenFOAM-based dispersion simulations to run ensemble simulations for probabilistic explosion assessment

Questions?