Engineering Models for Vented Lean Hydrogen Deflagrations

Anubhav Sinha, Vendra Chandra and Jennifer X. Wen

Warwick FIRE, School of Engineering

University of Warwick, UK

Outline

- Introduction
- Review of Engineering Models
- Performance Evaluation of Engineering Models
- Effect of Obstacles
- HySEA Experiments – GexCon 20-feet ISO containers
- New Model development
- Concluding Remarks

Introduction

- Vented deflagrations – simplest way to relieve pressure
- Experiments are expensive, specially for large enclosures / buildings
- Computational models – challenge to incorporate large range of scales involved, time taking and large computational resources required
- EM – reasonable predictions, simple and fast to use
- Review Engineering models to assess their applicability for hydrogen deflagrations

Review of Engineering Models

These models are reviewed and their applicability is tested with experimental results available in literature and from results generated in this project

- EN14994 (2007)[1]
- NFPA 68 (2013)[2]
- Bauwens et al. (2012)[3]
- Molkov and Bragin (2015)[4]

[1] *EN 14994 (2007). Gas explosion venting protective systems*
[2] *NFPA 68. (2013): Standard on explosion protection by deflagration venting, 2013 Edition, National Fire Protection Association, Quincy, MA 02269.*
[3] *Bauwens, C. R., Chao, J., & Dorofeev, S. B. (2012). Effect of hydrogen concentration on vented explosion overpressures from lean hydrogen–air deflagrations. International journal of hydrogen energy.*
[4] *Molkov, V., Bragin, M. (2015). Hydrogen–air deflagrations: Vent sizing correlation for low-strength equipment and buildings. International Journal of Hydrogen Energy, 40(2), 1256-1266.*

EN14994 (2007)[1]

- The formulation is divided into two parts, one for a compact enclosure (with $L/D \leq 2$) and the other for elongated enclosure (with $L/D > 2$)
- A gas explosion constant KG which denotes maximum value of pressure rise per unit time is used to determine overpressure
- The constant KG is determined experimentally
- Effect of initial turbulence is not taken into account
- Not recommended for Hydrogen

NFPA 68(2013)[2]

- This model consists of two formulations – one for low static pressure and another for high static pressure
- Effect of turbulence on flame speed is accounted in this model formulation.
- Different considerations are given to the vent deployment, whether it is a part of a wall or a complete side wall is used as a vent
- In general, predictions from this model are conservative and tend to predict higher overpressures than experimentally obtained values

Bauwens et al.[3] Model

- This model is based on the multi-peak behaviour of vented explosions due to various physical processes involved
- Different formulations are give to derive maximum pressure for each peak
- Three different pressure peaks considered are –
    - External explosion (P1)
    - Flame-Acoustic interaction (P2)
    - Pressure peak due to presence of obstacles (P3)
- The maximum value of all these peaks gives the final overpressure value

Molkov and Bragin[4] Model

- This model is based on the novel concept of Deflagration-Outflow Interaction (DOI) number
- The major assumption is that the overpressure correlates with the DOI number and can be related using the turbulent Bradley number
- Various physical processes including initial turbulence, effect of elongated enclosure, effect of obstacles, fractal nature of flame-front, are accounted for in this model.
- Two formulations are proposed – one for conservative estimate and other for best fit value

Experimental Studies

These experimental studies are used to assess engineering models

	Geom	Vol (m3)	Vent Area (m2)	Fuel	Conc (%)	Ignition	Obs	Remarks
Kumar (2006) [5]	Cuboid	120	0.55/1.09/2.19	H2	8.5-12.0	BW	No	Initial Turb
Kumar (2009) [6]	Cuboid	120	0.55/1.09/2.19	H2	5.9-10.8	BW	No	Initial Turb
Daubech et al. (2011) [7]	Cyl	1/ 10.5	0.15 / 2	H2	10.0-27.0	BW	No	High L/D
Bauwens et al. (2012) [3]	Cube	63.7	5.4/ 2.7	H2	12.1-19.7	CI, BW, FW	Yes	
Schiavetti, and Carcassi (2016) [8]	Cube	25	1.004	H2	7.5-12.5	BW, cube centre	Yes	Obstacles

[5] *Kumar, K., Vented combustion of hydrogen-air mixtures in a large rectangular volume. In 44th AIAA Aerospace Sciences Meeting and Exhibit, 2006.*

[6] *Kumar, R. K. (2009). Vented Turbulent Combustion of Hydrogen-Air Mixtures in A Large Rectangular Volume. In 47th AIAA aerospace sciences meeting including the new horizons forum and aerospace exposition. Paper AIAA 2009-1380.*

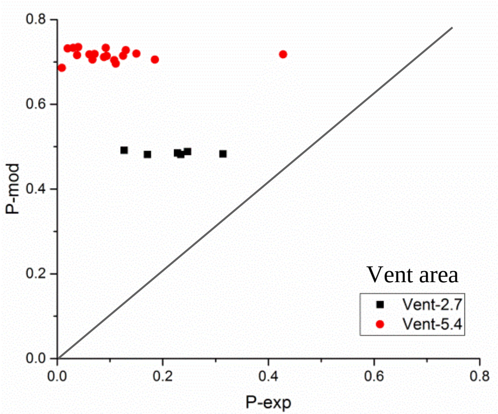
[7] *Daubech, J., Proust, C., Jamois, D., Leprette, E. (2011, September). Dynamics of vented hydrogen-air deflagrations. In 4. International Conference on Hydrogen Safety (ICHS 2011)*

[8] *Schiavetti, M., and M. Carcassi. "Maximum overpressure vs. H 2 concentration non-monotonic behavior in vented deflagration. Experimental results." International Journal of Hydrogen Energy (2016).*

EN14994 Model (2007)[1]

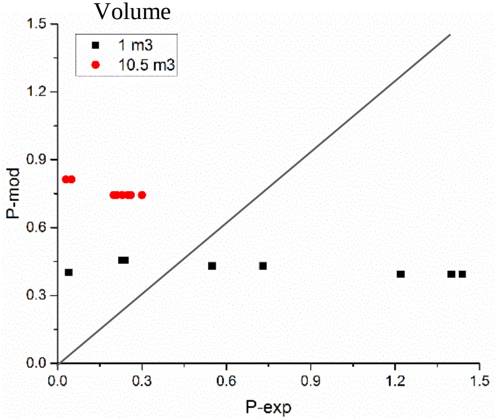
- Mixture composition is accounted for the factor KG (for compact enclosures)
- For a given geometry and comparable fuel concentration, vent area is dominant factor
- Data points are clustered as it gives similar prediction for fixed vent size

Line shows y = x



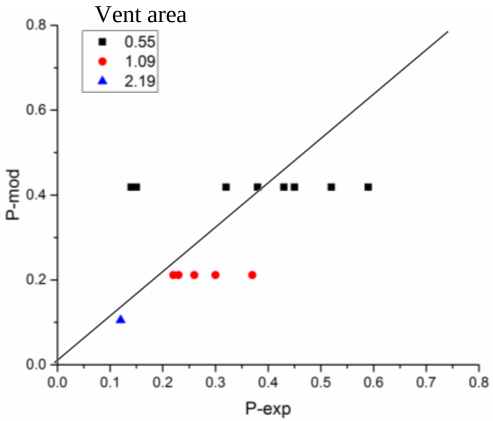
Predictions for Bauwens et al. (2012) experiments[3]

- Cubical enclosure - 63.7 m^3
- Includes cases **with obstacles**



Predictions for Daubech et al. (2011) experiments[7]

- Two cylindrical enclosures - 1 m^3 and 10.5 m^3
- **No obstacles**

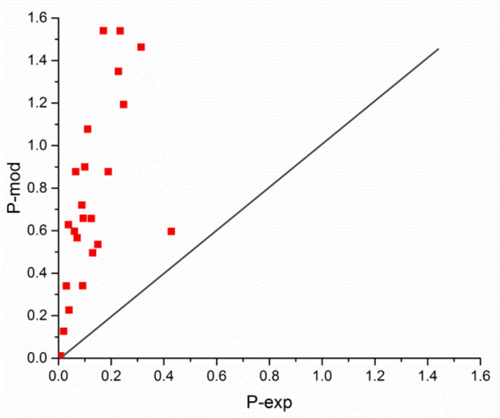


Predictions for Kumar (2009) experiments[6]

- Cubical enclosure - 120 m^3
- **No obstacles**

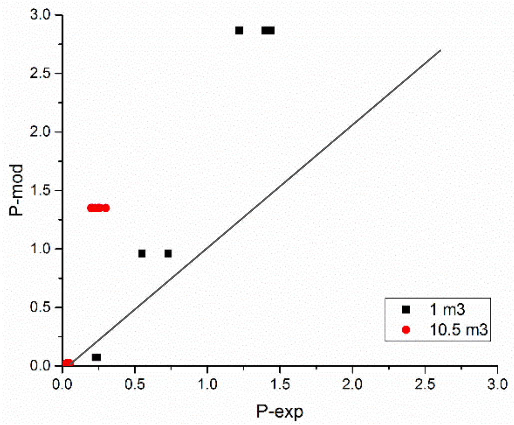
NFPA 68 Model (2013)[2]

- Over-prediction for most data points (conservative estimate) for various experimental results



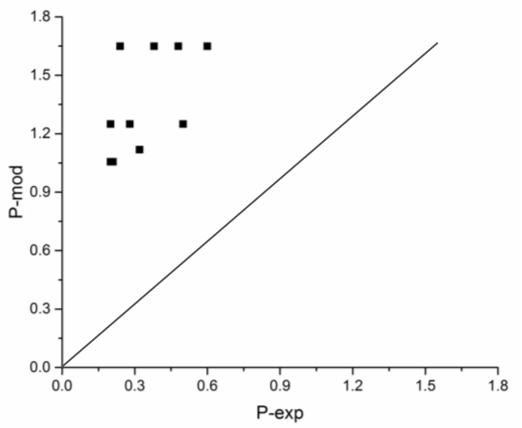
Predictions for Bauwens et al. (2012) experiments[3]

- Cubical enclosure - 63.7 m^3
- Includes cases **with obstacles**



Predictions for Daubech et al. (2011) experiments[7]

- Two cylindrical enclosure - 1 m^3 and 10.5 m^3
- **No obstacles**

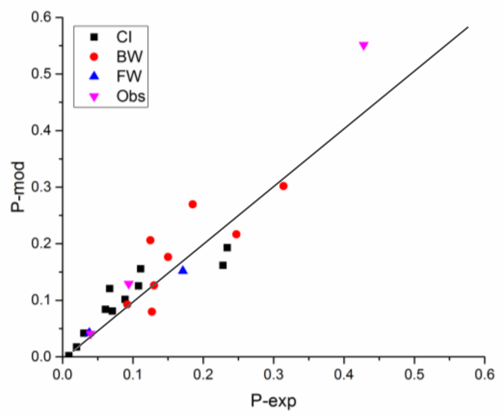


Predictions for Kumar (2006) experiments[5]

- Cubical enclosure - 120 m^3 – (L/D = 2.5)
- **No obstacles**

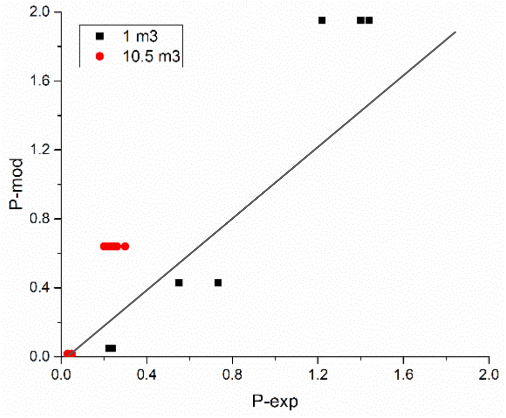
Bauwens et al. Model (2012)[3]

- Accounts for several physical aspects- calculates multiple peak pressures
- Under-prediction for Kumar's experiments – cases with high initial turbulence and high L/D (2.5)
- Some experiments of Daubech et al. (2011) also show high over-prediction (L/D=3.3)



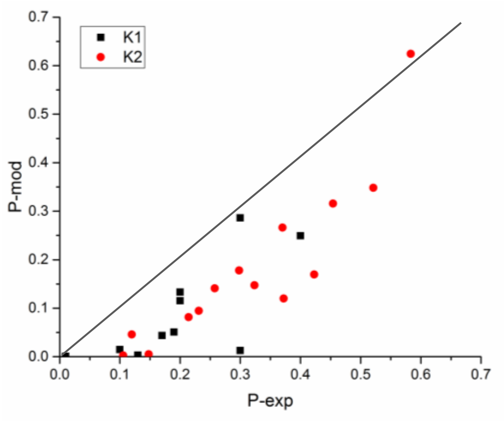
Predictions for Bauwens et al. (2012) experiments[3]

- Cubical enclosure - 63.7 m^3
- Includes cases **with obstacles**



Predictions for Daubech et al. (2011) experiments[7]

- Two cylindrical enclosure - 1 m^3 and 10.5 m^3
- **No obstacles**

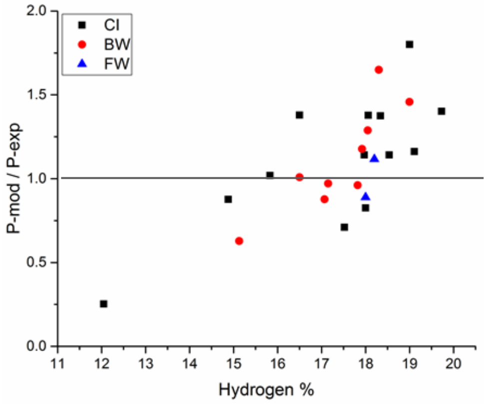


Predictions for Kumar's experiments[5,6]

- Cubical enclosure - 120 m^3 – (L/D = 2.5)
- **No obstacles**

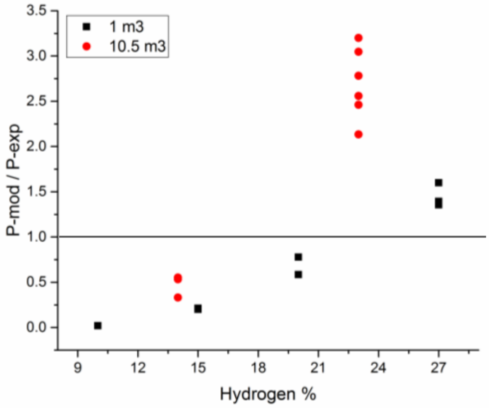
Bauwens et al. Model (2012)[3]

- Under-predicts cases with Forward wall ignition
- Over-predicts for larger enclosure used by Daubech et al. (L/D=3.3) – for higher H_2 concentrations



Predictions for Bauwens et al. (2012) experiments[3]

- Cubical enclosure - 63.7 m^3
- Includes cases **with obstacles**

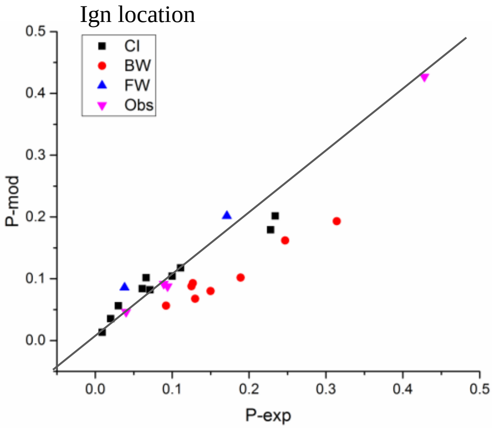


Predictions for Daubech et al. (2011) experiments[7]

- Two cylindrical enclosures - 1 m^3 (L/D = 1.4) and 10.5 m^3 (L/D = 3.3)
- **No obstacles**

Molkov and Bragin Model (2015)[4]

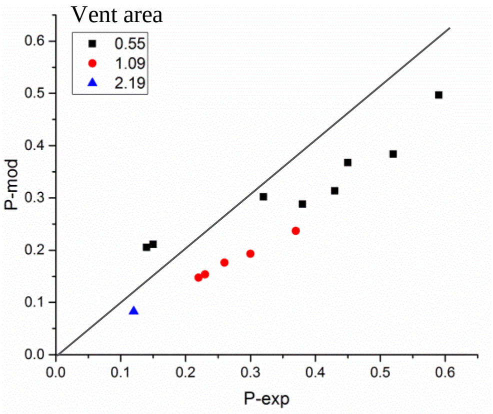
- In the formulation, two equations are suggested – conservative and best-fit
- Best-fit formula appears to slightly under-predict for most of data points



Predictions for Bauwens et al. (2012) experiments[3]

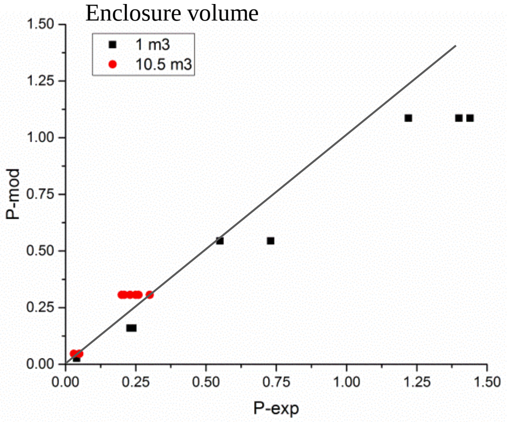
- Cubical enclosure - 63.7 m^3
- Includes cases **with obstacles**

▪ For obstacles, Ξo is provided in Molkov and Bragin[4] (3.5 for BW and 1.0 for CI)



Predictions for Kumar (2009) experiments[6]

- Cubical enclosure - 120 m^3
- **No obstacles**

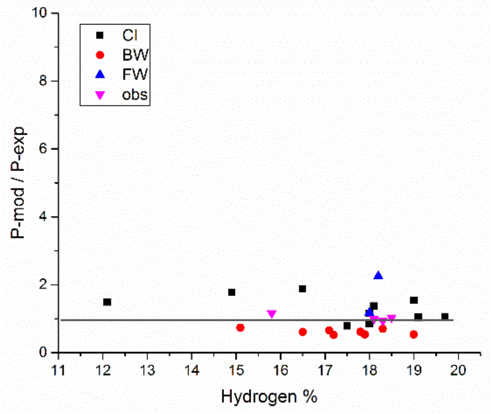


Predictions for Daubech et al. (2011) experiments[7]

- Two cylindrical enclosures - 1 m^3 and 10.5 m^3
- **No obstacles**

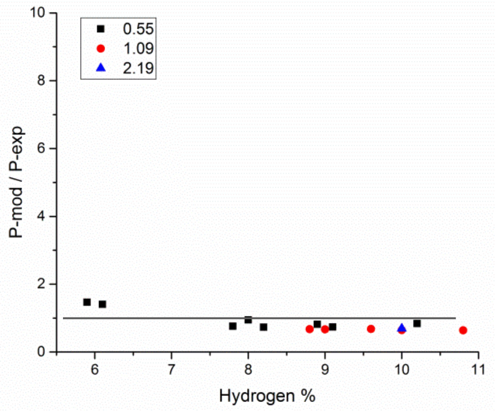
Molkov and Bragin Model (2015)[4]

- The predictions appear to be reasonable for the experiments compared
- The formulation of coefficient for obstacles is not clearly defined



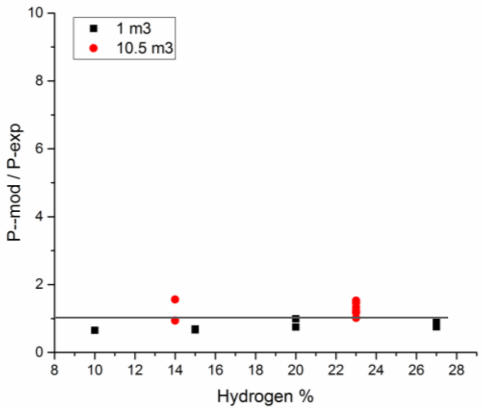
Predictions for Bauwens et al. (2012) experiments[3]

- Cubical enclosure - 63.7 m^3
- Includes cases **with obstacles**



Predictions for Kumar (2009) experiments[6]

- Cubical enclosure - 120 m^3
- **No obstacles**



Predictions for Daubech et al. (2011) experiments[7]

- Two cylindrical enclosures - 1 m^3 and 10.5 m^3
- **No obstacles**

- For obstacles, Ξo is provided in Molkov and Bragin[4] (3.5 for BW and 1.0 for CI)

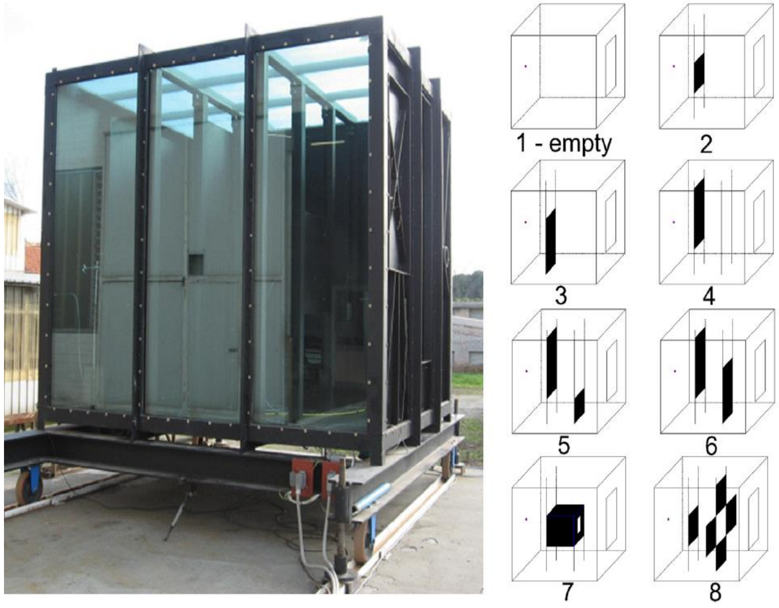
Issues in Current models

- EN-14994 and NFPA – mostly over-predicting – will result in a very large / unfeasible vent area
- Models of Bauwens et al. and Molkov and Bragin have many equations and not simple to implement.
- No formulation for stratified fuel distribution which resembles realistic accidental cases rather closely
- Effect of obstacles need to be investigated further and more accurate models are required
- Hydrogen flame speed is much higher than hydrocarbons and same formulations will not necessary be correct to use.

Effect of Obstacles

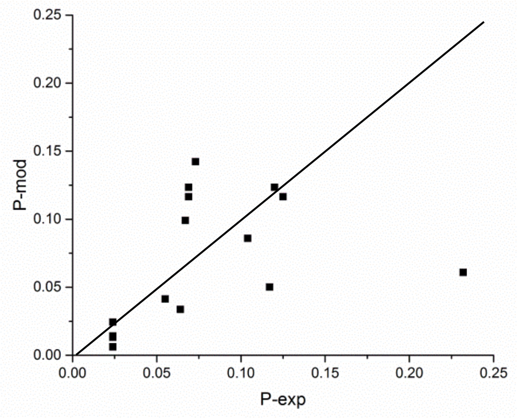
Obstacles

- Scarcity of data on systematic study of effect of obstacles
- Schiavetti and Carcassi (2016) [8] – impact of obstacles in a small volume enclosure
- Flat plates are used as obstacles
- More such experiments required for realistic obstacles in a larger geometry

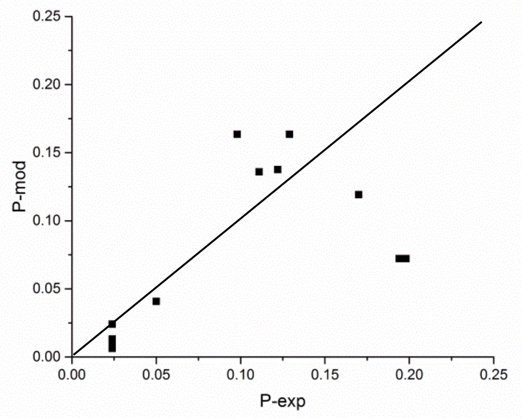


(Schiavetti and Carcassi (2016))[8]

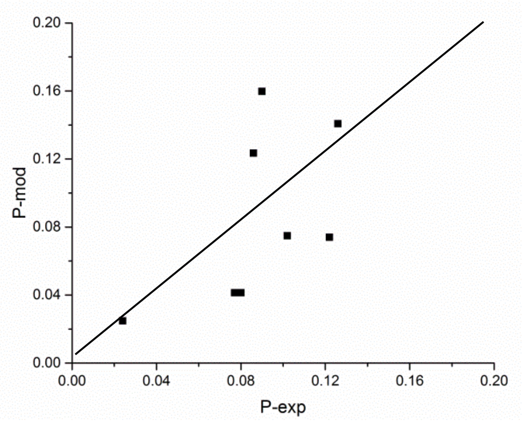
Obstacles -Bauwens et al. Model (2012)[3]



Obstacle 2



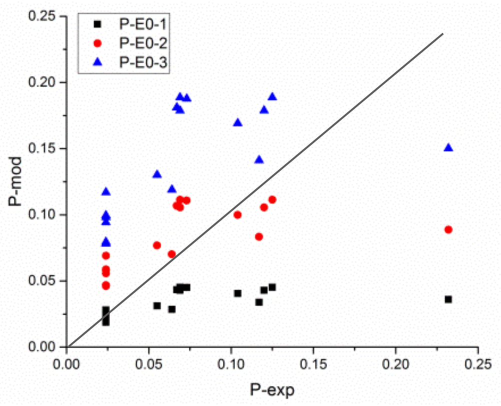
Obstacle 3



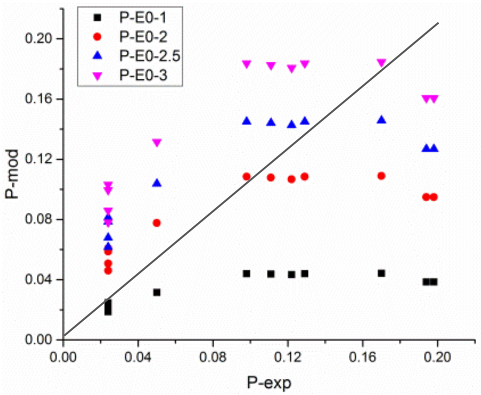
Obstacle 4

- Predictions are reasonably close to experiments with some scatter
- Prescribed formulation is used – no new addition for these cases

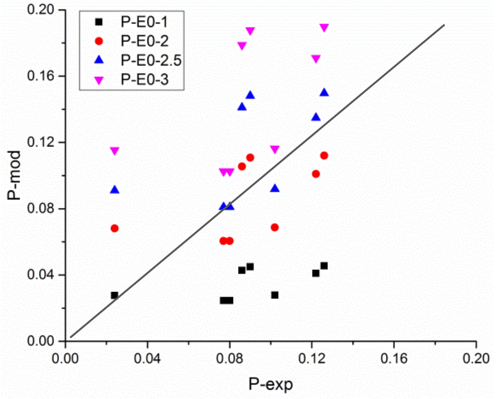
Obstacles – Molkov and Bragin Model (2015)[4]



Obstacle 2



Obstacle 3



Obstacle 4

Obstacle config	Ξo (best fit)
Obs 2	**2.00**
Obs 3	**2.00**
Obs 4	**2.00**
Obs 5	**2.00**
Obs 6	**3.00**
Obs 8	**3.50**

- Different values of Ξo used and plotted with various obstacle configurations
- The best fit value of Ξo is shown in table

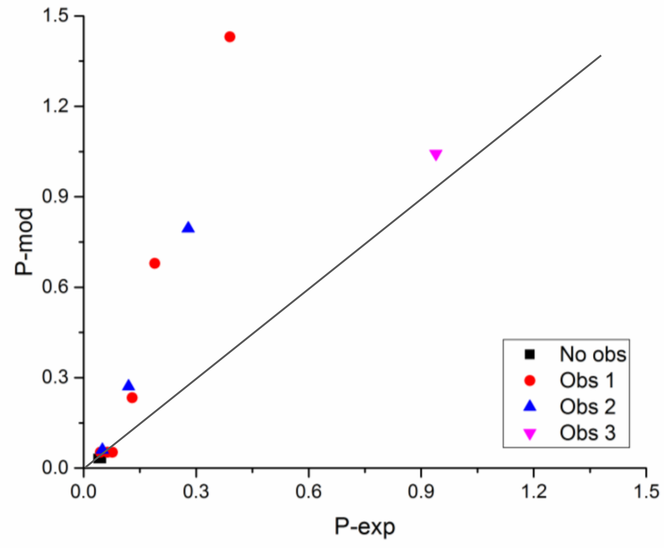
HySEA Experiments -
GexCon (20 feet ISO containers)

Experiments with ISO 20 feet container

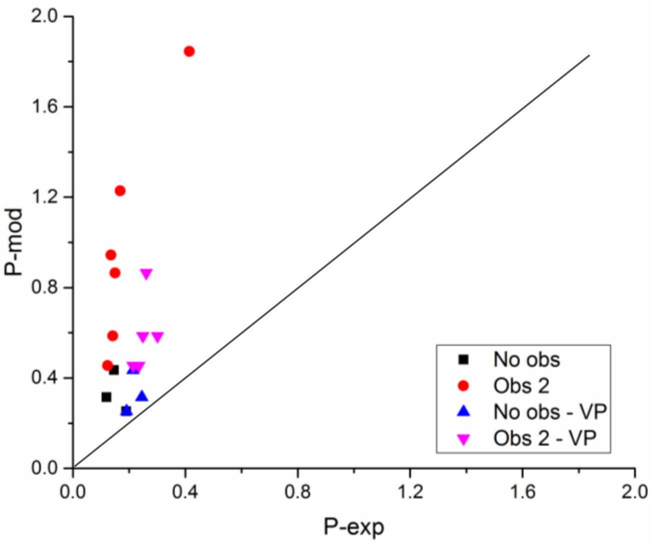
Venting through door

Venting through roof

Bauwens et al. Model (2012)[3]



Venting through door



Venting through roof

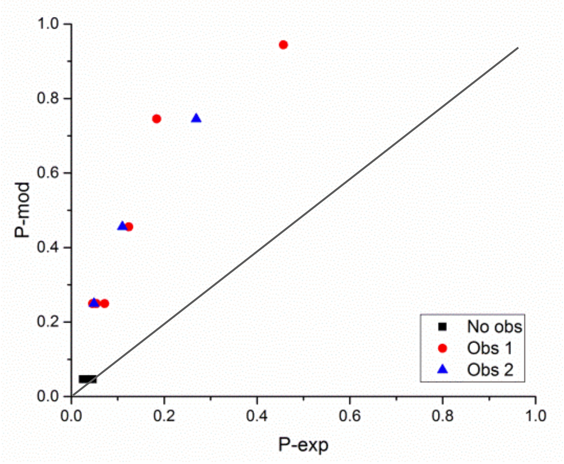
Obs 1 – Bottle
Obs 2 – Pipe rack
Obs 3 – Bottle + Pipe rack

- Cubical enclosure – 33 m^3
- Includes cases **with obstacles**

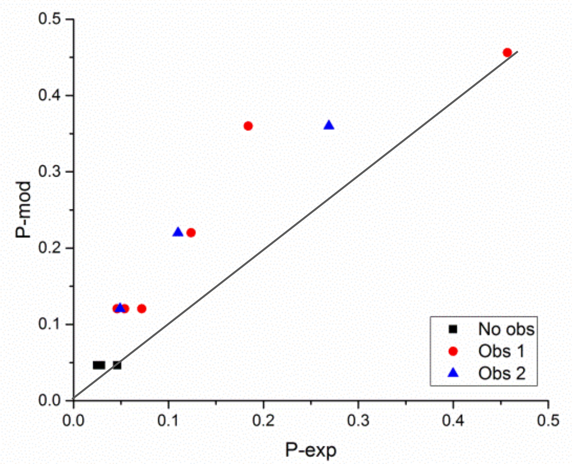
Bauwens et al. (2012) model[3]

- Over-prediction is observed for cases with obstacles for both experimental sets

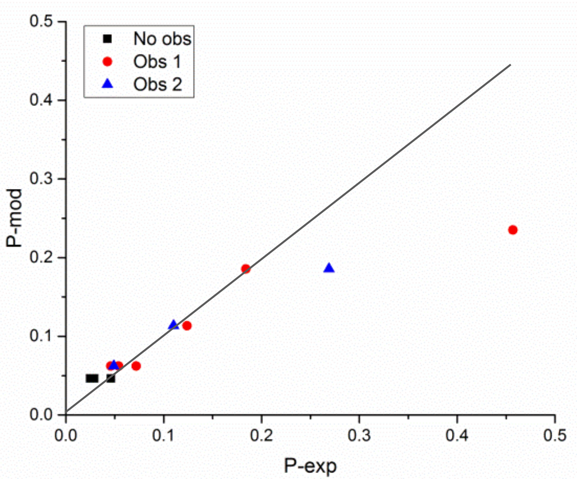
Molkov and Bragin Model (2015)[4]



Ξo = 3.5



Ξo = 2.0

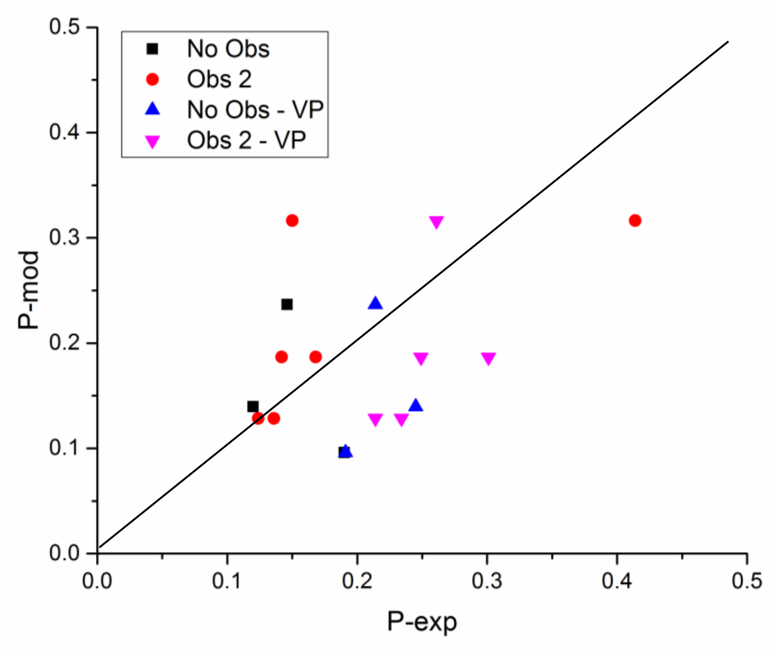


Ξo = 1.25

Venting through door

Obs 1 – Bottle
Obs 2 – Pipe rack
Obs 3 – Bottle + Pipe rack

Molkov and Bragin Model (2015)[4]



Venting through roof - Ξo = 1.25

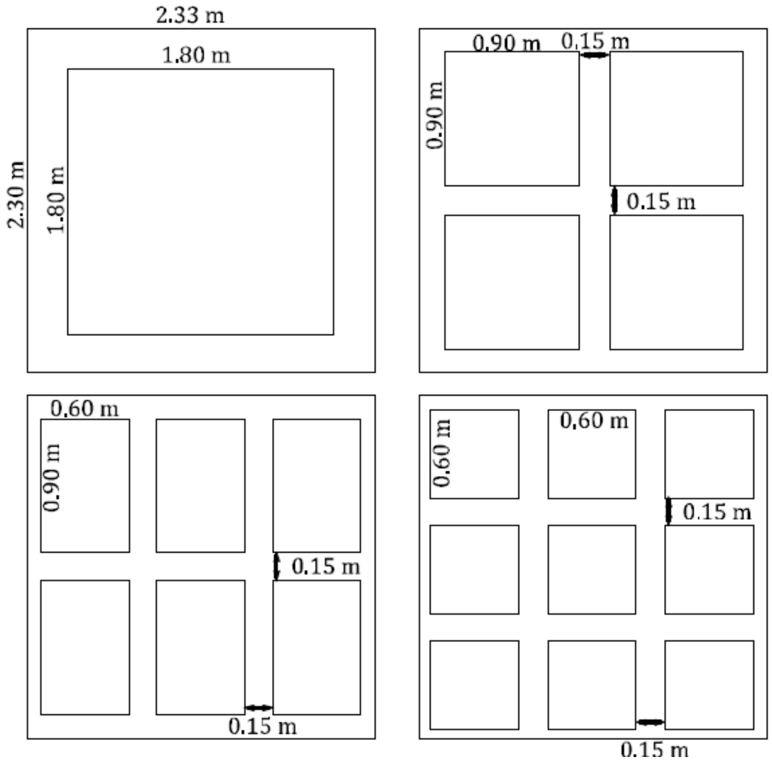
Blockage Ratio	Ξo	Experiments
0.06	3.50	Bauwens et al. (2012) - BW ignition
0.30	1.25	GexCon 20 ft ISO container-bottles – BW
0.12	1.25	GexCon 20 ft ISO container -pipe and rack- BW

New Engineering Model

Expectation from new model for Hydrogen

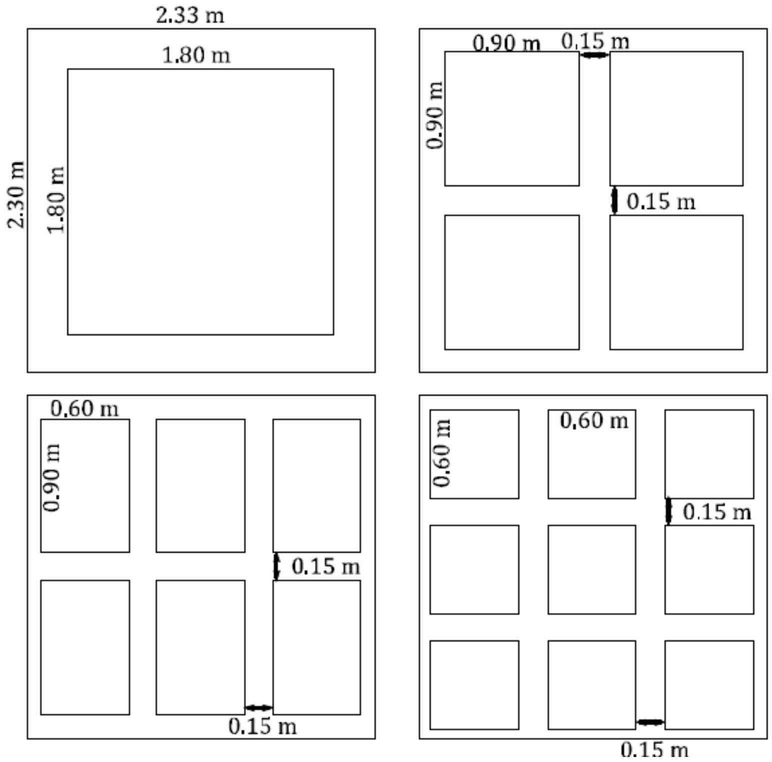
- Accurate prediction within acceptable limits
- Simple and easy to calculate formulas / equations
- Able to predict overpressure for cases with realistic accidental scenarios
    - Stratified fuel distribution
    - Presence of obstacles
- Consider unique properties of hydrogen into its formulation
    - Higher flame-speed
    - Increase in flame-speed, due to Lewis number effects and instability in lean mixtures

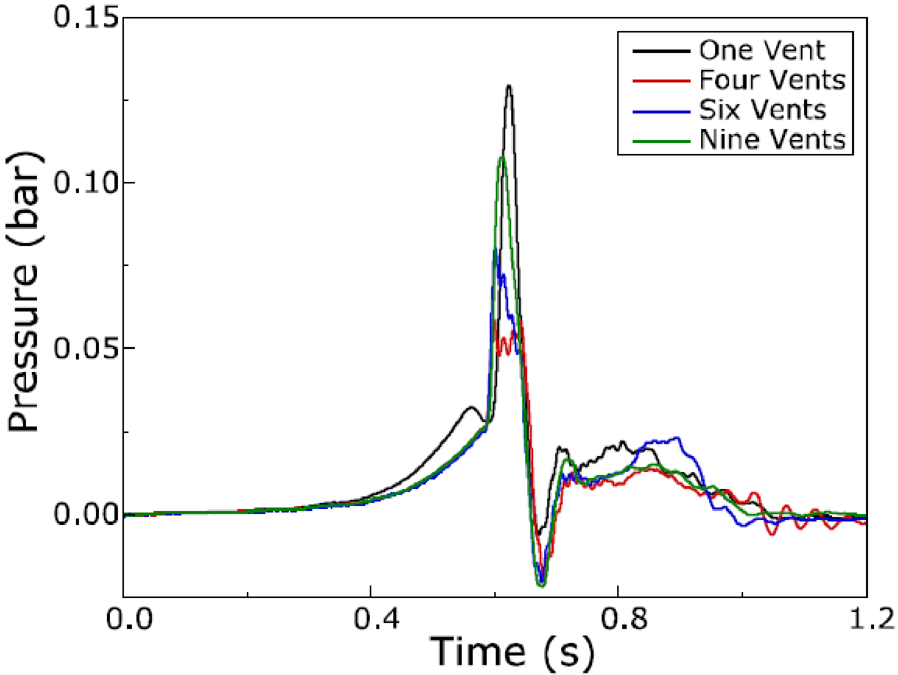
Same vent area gives same overpressure ?



Bauwens, C.R., and Dorofeev, S., Understanding the effect of multiple adjacent vent panels on explosion overpressures , in *ICDERS 2017*

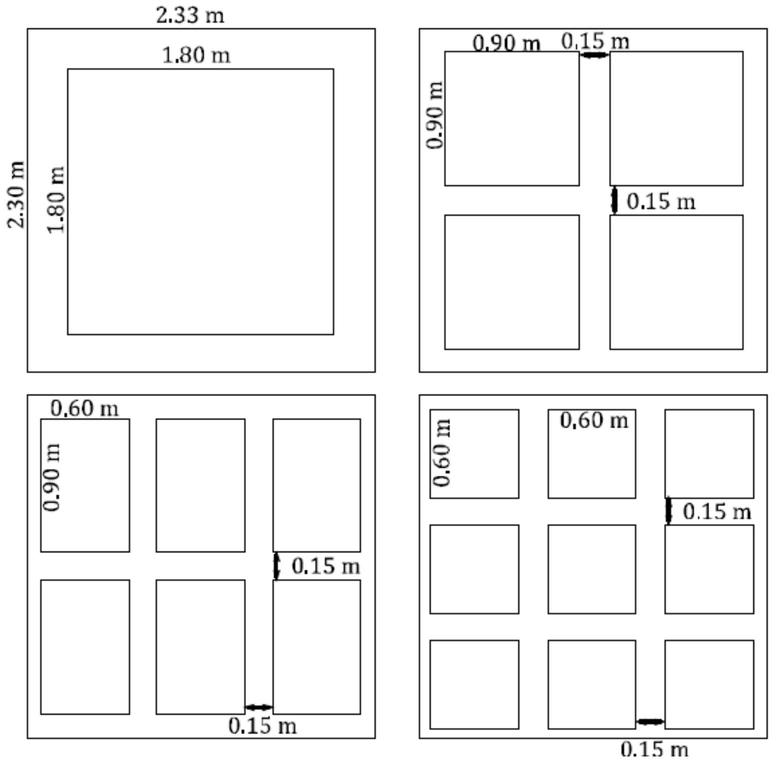
Same vent area gives same overpressure ?

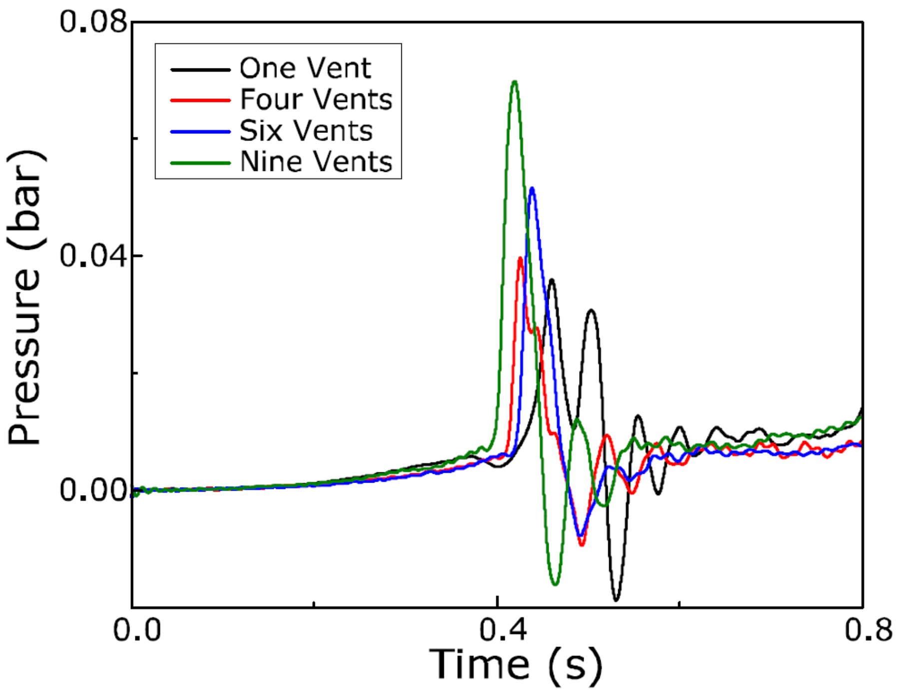




Back-wall Ignition

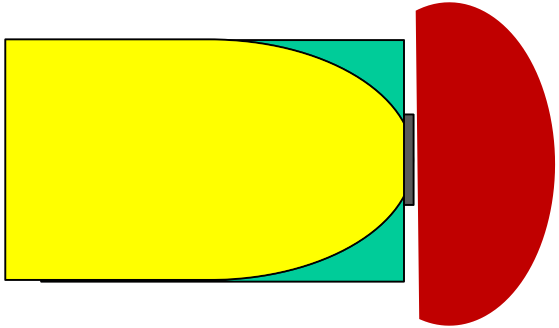
Same vent area gives same overpressure ?





Central Ignition

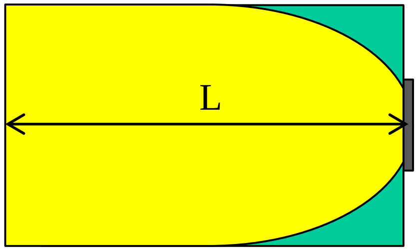
New model development



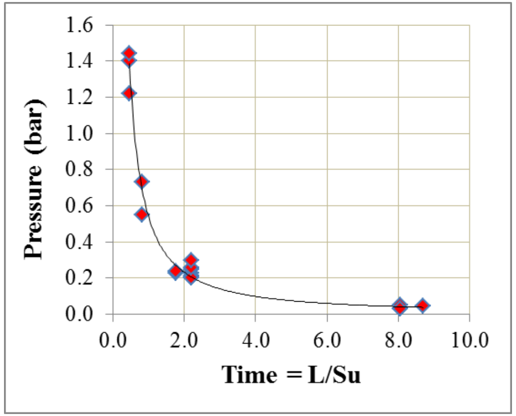
- The internal flame reaches the vent panel and ignites the external cloud
- External explosion acts as restriction at the vent and results in pressure rise inside enclosure
- The vent acts an orifice and fluid suffer a pressure drop in flowing through it.
- Pressure generated by external explosion has to be determined accurately

External Explosion

- Mixtures with higher flame-speed result in higher peak pressures
- As the flame in the enclosure ignites the external cloud, the time required for flame to reach the vent should affect overpressure
- External cloud is formed by unburnt gas jet coming out of the vent.
- Spread and stratification of this cloud will determine the overpressure



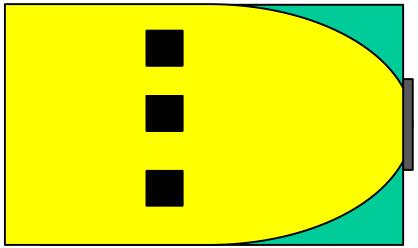
Time = L / Su

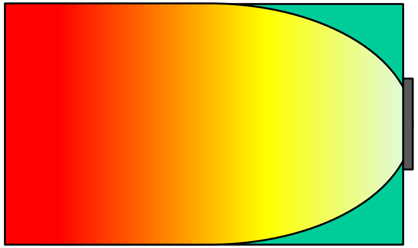


Results from Daubech et al. (2011) experiments[7]

Obstacles and Stratified Mixture

- Obstacles
  - reduce available cross section,
  - increase flame surface area
  - increase flame speed
- Stratified Mixture – increases flame speed
  - equivalent mixture composition
  - 1-D integration if concentration profile is available
- Both these parameters affect time for flame-front to reach vent and ignite external cloud





Present Effort

- Calculation of the cloud ignition time
- Understanding the cloud structure, spread and stratification – pressure generated
- Calculating the overpressure generated inside the enclosure using the external overpressure
- Integrate effect of obstacles and stratified mixture distribution into this model

Concluding remarks

- Both NFPA 68 and EN 14994 models over-predicted the experimental measurements
- The predictions of Bauwens et al. (2012) model and Molkov and Bragin (2015) model (without obstacles) are in reasonable agreement with the experimental data, but both models have some limitations:
  - The predictions of Bauwens et al. (2012) model have relatively large discrepancy for high L/D enclosures and cases with high initial turbulence
  - Molkov and Bragin (2015) model does not provide any specific treatment for obstacles. Instead obstacles can only be considered through adjusting the coefficient Ξo
  - Neither considers stratified distribution of the fuel
- New model using external cloud combustion is under development

Acknowledgements

- The HySEA project is supported by the Fuel Cells and Hydrogen 2 Joint Undertaking (FCH 2 JU) under the Horizon 2020 Framework Program for Research and Innovation.

- We also thank Regis Bauwens (FM Global) and Trygve Skjold (GexCon) for useful discussions and suggestions

Thank You