IA HySafe Research Priorities Workshop on Hydrogen Safety

26-27 September 2016, Petten, the Netherlands

Research progress, near term research directions, and gaps of knowledge

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Acknowledgements

HySAFER team

- Dr Sile Brennan
- Dr Volodymyr Shentsov
- Dr James Keenan
- Dr Sergii Kashkarov
- Dr Yangkyun Kim
- Dr Wookyung Kim

Research projects

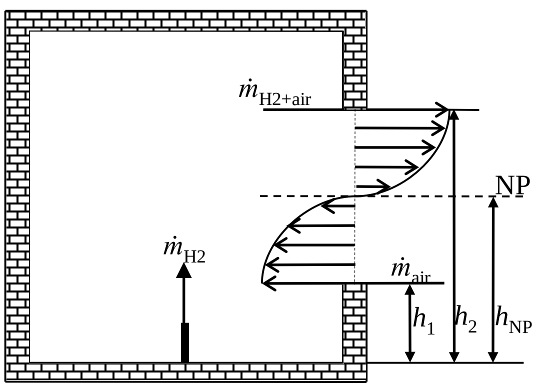
- EC H2FC Research Infrastructure
- FCH-JU HyIndoor
- FCH-JU HyResponse
- UK EPSRC H2FC SUPERGEN Hub
- UK EPSRC H2FC SUPERGEN Challenge

Progress : releases

Natural vs passive ventilation for single vent

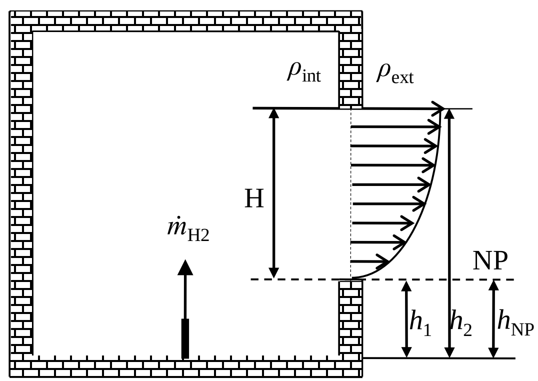
Fixed neutral plane

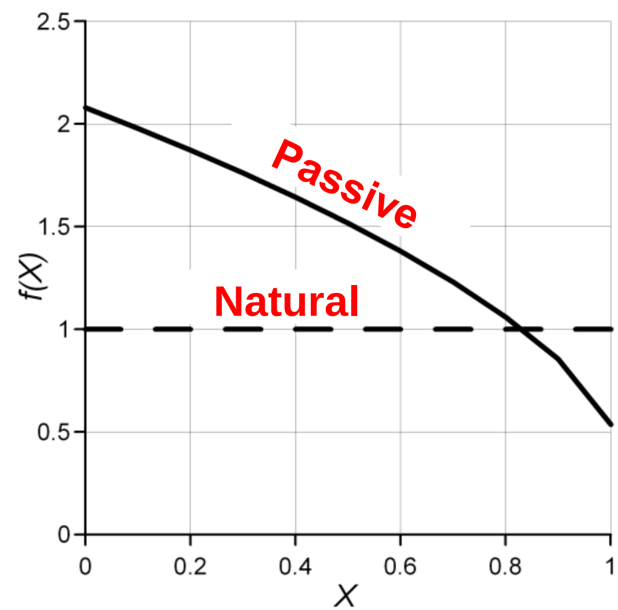
$$X = \left[\frac{Q_0}{C_D A (g' H)^{1/2}}\right]^{2/3}$$



Variable neutral plane

$$X = f(X) \cdot \left[\frac{Q_0}{C_D A (g' H)^{1/2}}\right]^{2/3}$$





Difference:

$$f(X) = \left(\frac{9}{8}\right)^{1/3} \cdot \left\{ \left[1 - X\left(1 - \frac{\rho_{H_2}}{\rho_{air}}\right)\right]^{1/3} + (1 - X)^{2/3} \right\}$$

Natural ventilation

- Underestimate x2 (lean)
- Overestimate x2 (rich)

Example

- Natural 3.5% v/v < LFL
- Passive > 7% v/v > LFL

Molkov V., Shentsov V., Quintiere J. “Passive ventilation of a sustained gaseous release in an enclosure with one vent”, *Int. J. Hydrog. Energy*, vol. 39, pp. 8158-8168, 2014

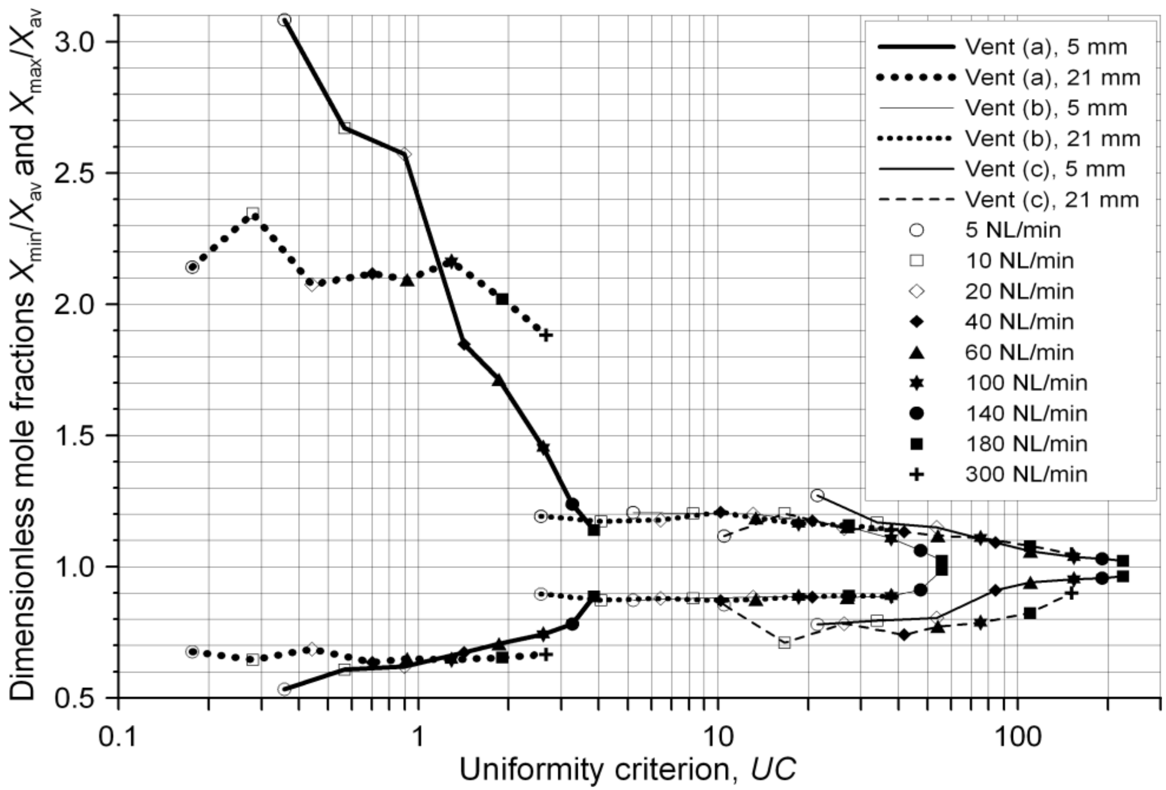
Progress: releases

Passive ventilation for single vent

Criterion for uniformity

$$UC = \frac{V^{2/3}\sqrt{D}}{A\sqrt{H}} \frac{\dot{m}_{ent}(x)}{\dot{m}_{mix}} \qquad \dot{m}_{ent}(x) = K_1 M_0^{1/2} \rho_{mix}^{1/2} x$$

$$\dot{m}_{mix} = \dot{m}_{H2} + \dot{m}_{air}$$



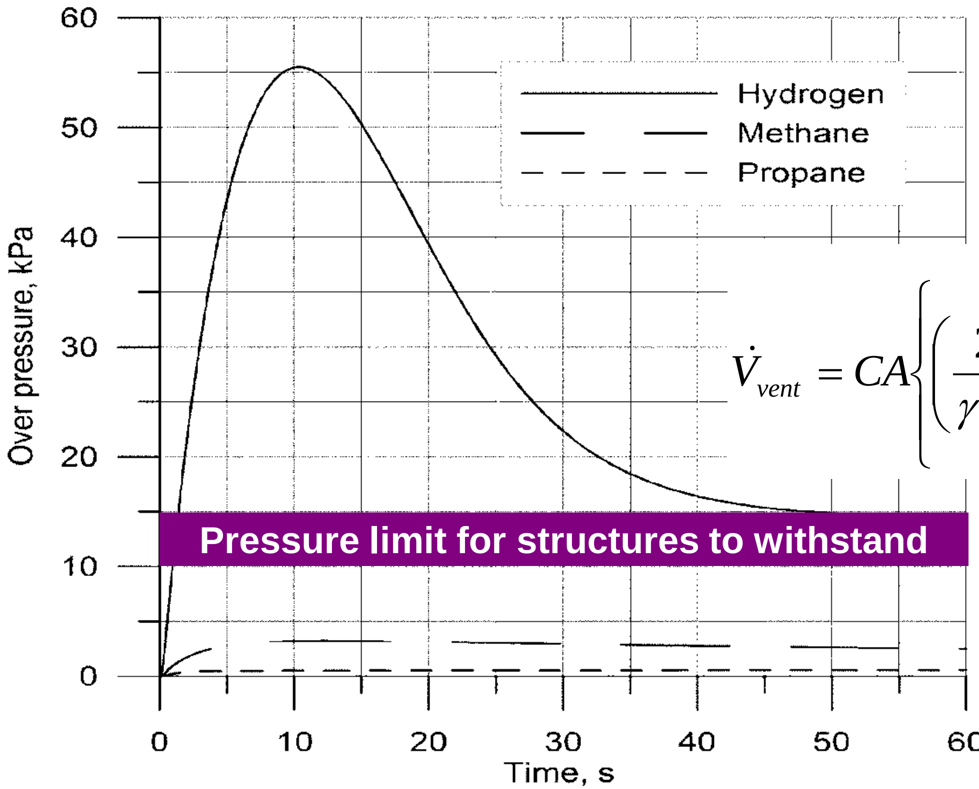
Molkov V., Shentsov V., Quintiere J. “Passive ventilation of a sustained gaseous release in an enclosure with one vent”, *Int. J. Hydrog. Energy*, vol. 39, pp. 8158-8168, 2014

Progress : releases

PPP for non-reacting release

Example of pressure peaking phenomenon (PPP) for non-reacting release:

- Garage *LxWxH*=4.5x2.6x2.6 m, “brick” vent
- CGH2 storage: 350 bar, ∅5.08 mm orifice, mass flow rate 390 g/s

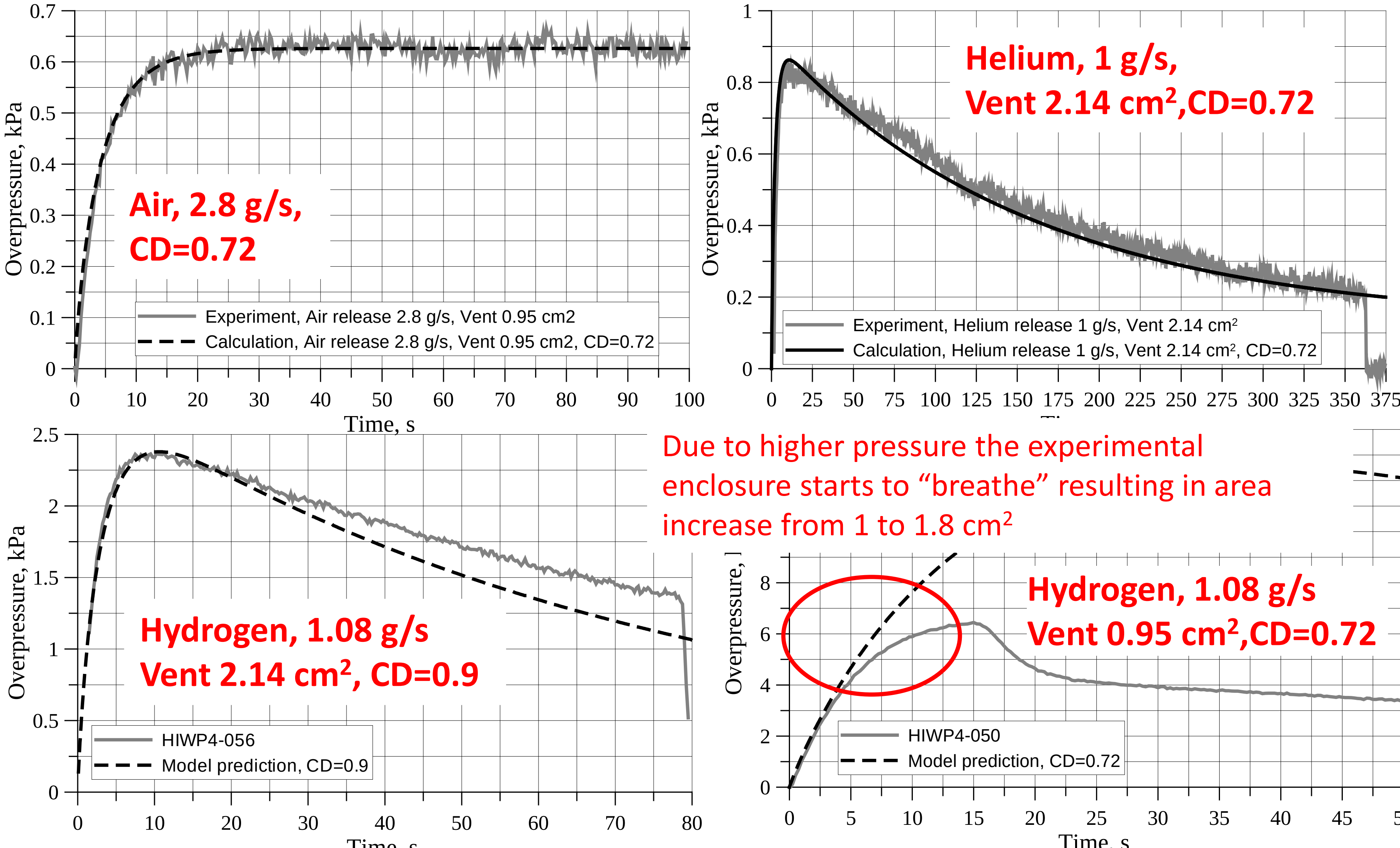


$$\dot{V}_{vent} = CA\left\{\left(\frac{2\gamma}{\gamma-1}\right)\frac{P_S}{\rho_{encl}}\left[\left(\frac{P_S}{P_{encl}}\right)^{\frac{2}{\gamma}} - \left(\frac{P_S}{P_{encl}}\right)^{\frac{\gamma+1}{\gamma}}\right]\right\}^{\frac{1}{2}}$$

S. Brennan and V. Molkov, “Safety assessment of unignited hydrogen discharge from onboard storage in garages with low levels of natural ventilation,” *Int. J. Hydrog. Energy*, vol. 38, no. 19, pp. 8159–8166, Jun. 2013.

Progress: releases

Validation of PPP model, non-reacting release

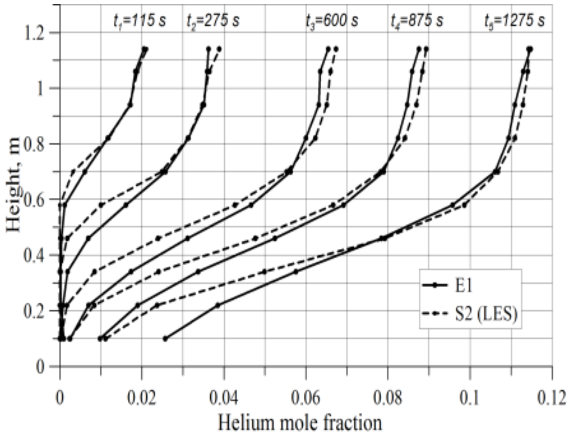


V. Shentsov, M. Kuznetsov, and V. Molkov, “The pressure peaking phenomenon: validation for unignited releases in laboratory-scale enclosure,” in *ICHS 2015*, Yokohama, Japan, 2015, vol. 148.

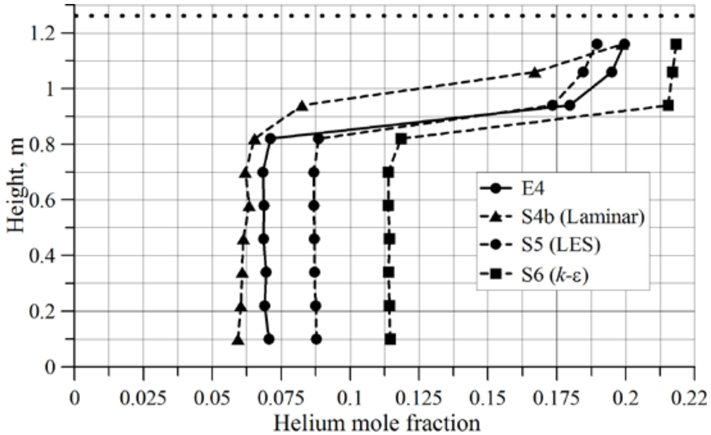
Progress: releases

LES of indoor releases

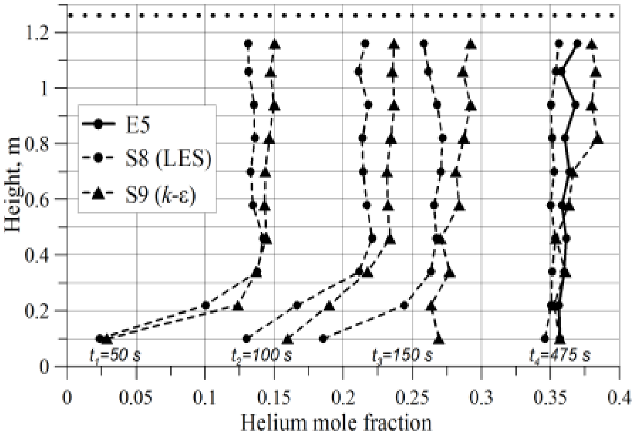
Laminar release
***Re*=39**



Transitional release
***Re*=2863**



Turbulent release
***Re*=6968**



Experiment: *Cariteau B., Tkatschenko I., Int.J.Hydrog.Energy, vol. 38, pp. 8030–8038, 2013*

LES performs best though range of release regimes (laminar to weakly turbulent)

- Laminar
  - LES reproduces laminar release and dispersion (when properly applied)
- Transitional
  - LES outperforms standard k-e model
- Turbulent
  - LES and k-e models reproduce weakly turbulent flow
  - laminar model - not applicable

Molkov V., Shentsov V. “Numerical and physical requirements to simulation of gas release and dispersion in an enclosure with one vent”, *Int. J. Hydrog. Energy*, vol. 39, no. 25, pp. 13328-13345, Aug. 2014.

Progress: jet fires

Regimes of indoor jet fires

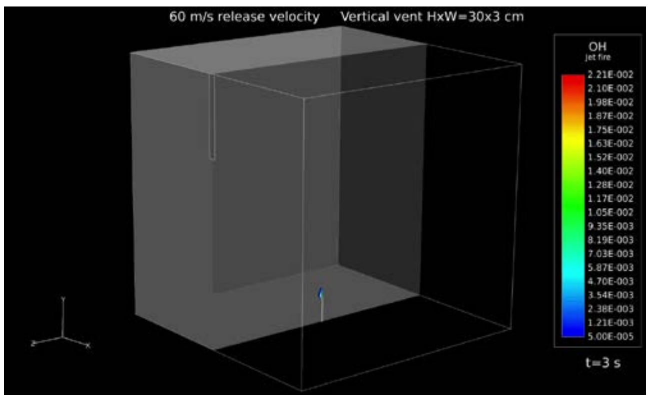
Fire regime vs. flow rate

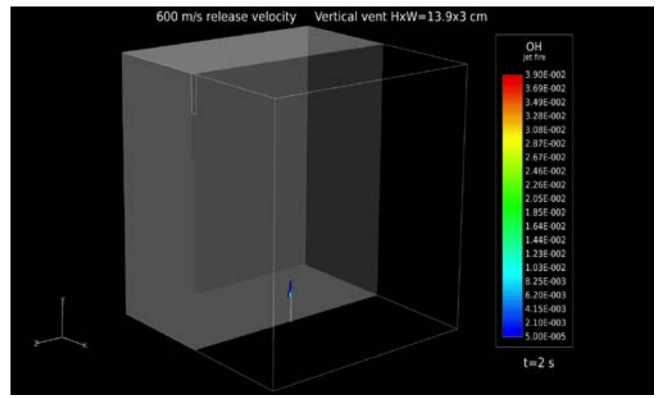
- Well ventilated fire (small leak rates)
- Under-ventilated fires
    - External flame (moderate flow rates)
    - Self-extinction (higher flow rates)
    - External flame (very high flow rate)

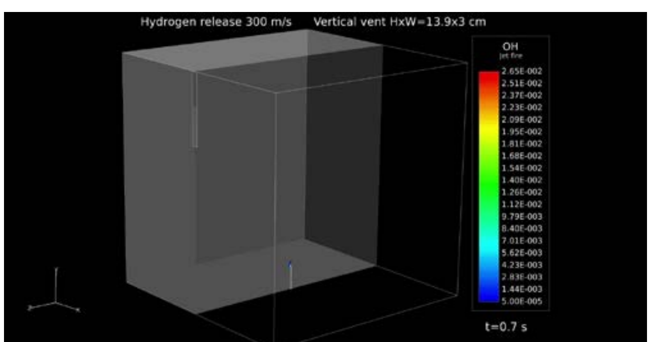
Need for detailed chemistry

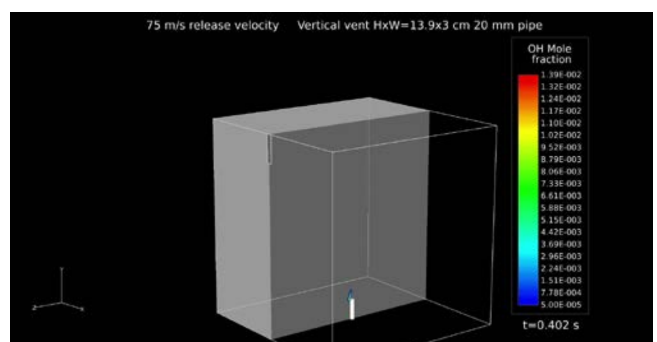
⇩

EDC combustion model









V. Molkov, V. Shentsov, S. Brennan, and D. Makarov, "Hydrogen non-premixed combustion in enclosure with one vent and sustained release: Numerical experiments," *Int. J. Hydrog. Energy*, vol. 39, no. 20, pp. 10788–10801, Jul. 2014.

Progress: blast waves

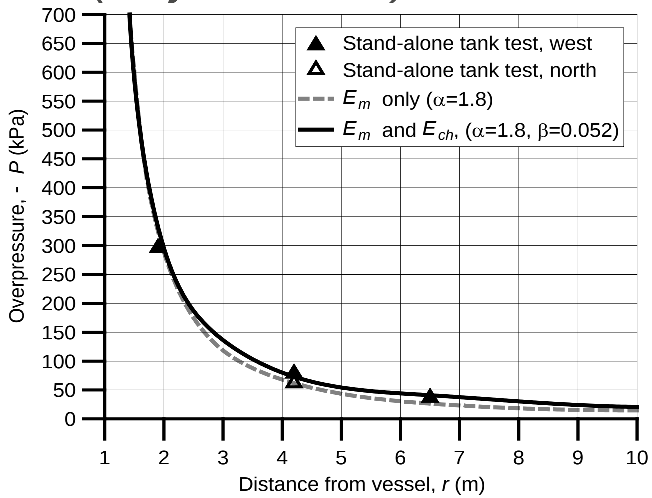
Analytical blast wave decay model

- Real gas EOS
- Chemical energy (H_2 combustion in air) added dynamically to hydrogen mechanical compression energy

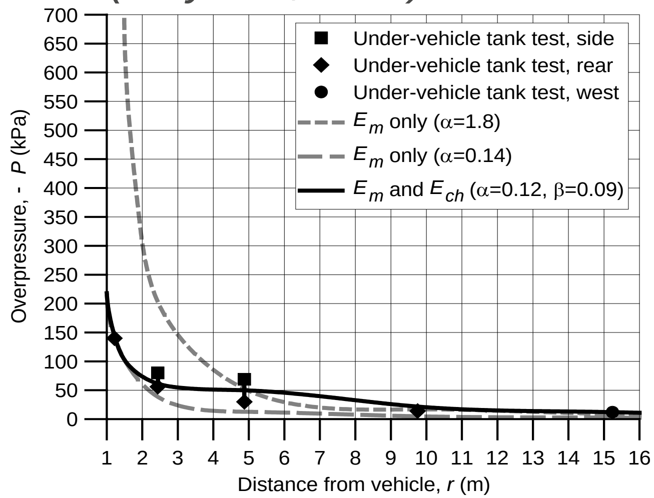
$$\Delta E_m = \frac{(p_g - p_s)\cdot(V - mb)}{\gamma - 1}$$

$$\bar{r}_P = r\left(\frac{p_s}{\alpha \cdot E_m + \beta \cdot \left(\frac{r_{sh}}{r_b}\right)^3 \cdot E_{ch}}\right)^{1/3}$$

Stand-alone tank rupture *(Weyandt, 2005)* validation



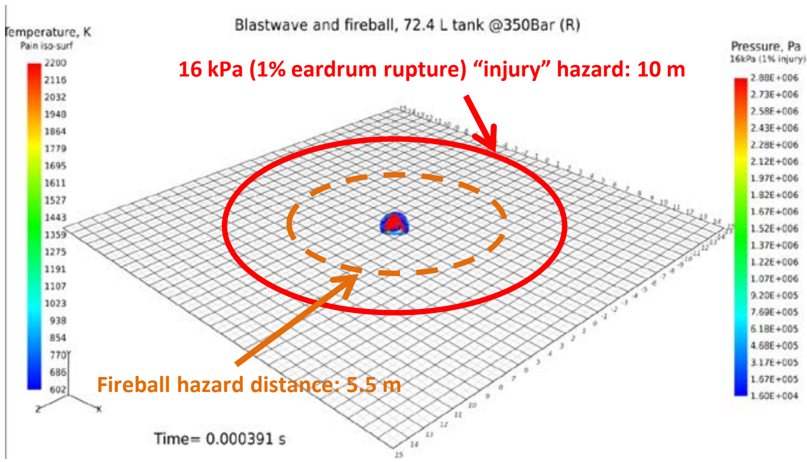
Under-vehicle tank rupture *(Weyandt, 2006)* validation



Molkov V., Kashkarov S. "Blast wave from a high-pressure gas tank rupture in a fire: standalone and under-vehicle hydrogen tanks", Proc. of 6th ICHS, 19-21 October 2015, Yokohama, Japan

Progress: blast waves

CFD of blast wave and fireball radiation (ideal gas)



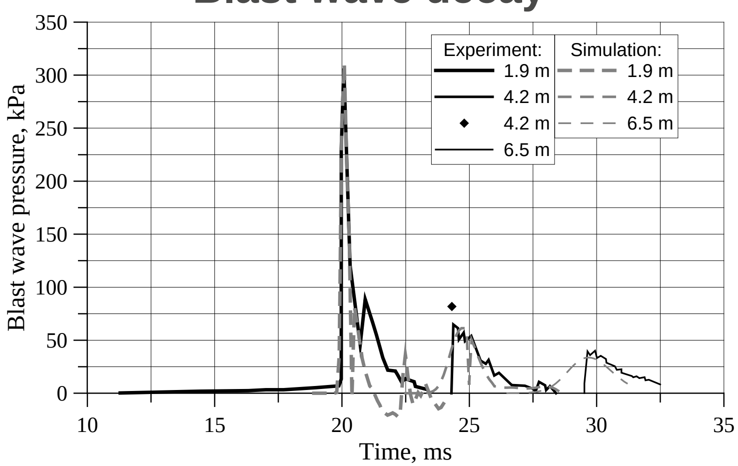
Domain

- Blast wave hemisphere: *R* = 50 m
- Fireball hemisphere: *R* = 10 m
- Tank hemisphere: *R* = 2 m
- Tank size *L*x*D*=0.66 × 0.37 m

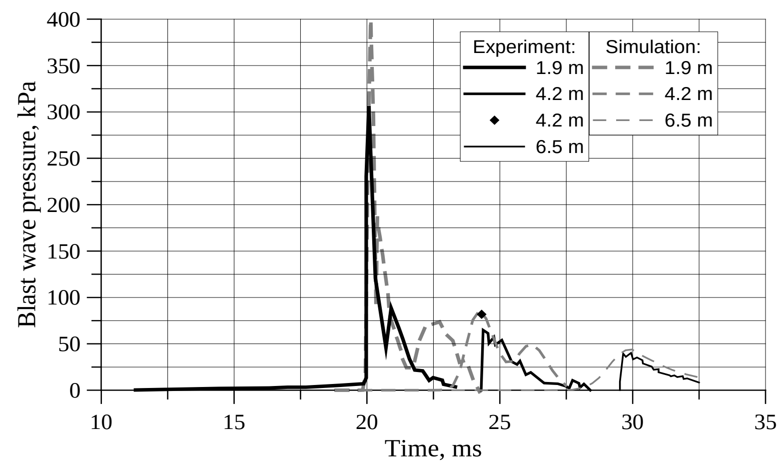
CFD model

- RNG k-ε turbulence model
- EDC combustion model, 37-steps chemistry, ISAT algorithm
- DO radiation model

Blast wave decay



- Overpressure transients (with radiation)



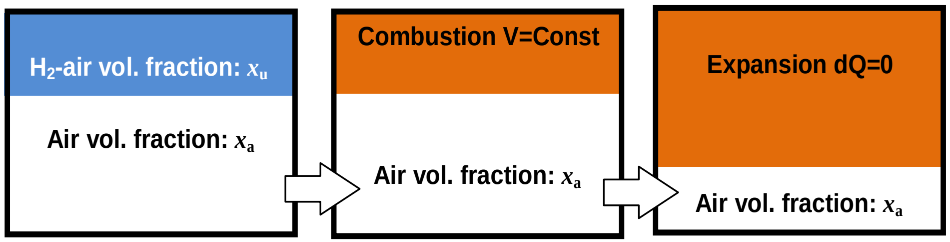
- Overpressure transients (no radiation)

Kim W., Shentsov V., Makarov D., Molkov V. "High pressure hydrogen tank rupture: blast wave and fireball", Proc. of 6th ICHS, 19-21 October 2015, Yokohama, Japan

Progress: deflagrations

Localised mixture deflagration (1)

Analytical model for maximum hydrogen inventory in a sealed enclosure



Initial parameters	Combustion V=Const	Expansion dQ=0
Initial state: T_0, p_0 H2: m_{H2} H2-air mixture: m_u, M_u, V_u Air: m_a, M_a, V_{a0}	Burnt mixture: m_b, T_{b1}, p_{b1} Air: m_a, M_a, T_0, p_0	Burnt mixture: m_b, T_{b2}, p_2 Air: m_a, M_a, T_{a2}, p_2

Analytical thermodynamic model for closed vessel deflagration:

$$p_2 = x_u p_{b1} \left(\frac{p_2}{p_{b1}} \right)^{\frac{\gamma_b - 1}{\gamma_b}} + x_a p_0 \left(\frac{p_2}{p_0} \right)^{\frac{\gamma_a - 1}{\gamma_a}}$$

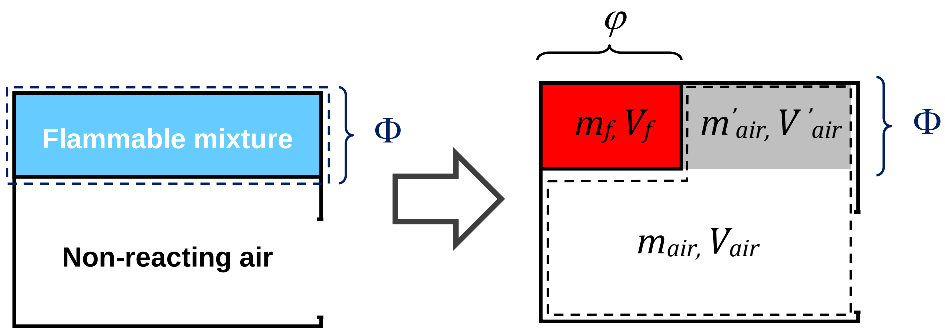
- Gives analytical expression for maximum overpressure in a closed space
- Validated against *Stamps D. et al., Proc. R. Soc. A, V.465, 2009*
- Allows to derive hydrogen inventory allowed to be released in closed space not to exceed a pressure threshold.
- For pressure threshold 10 kPa:

$$V_{H2}\left(m^3\right) < 0.00314 \cdot V\left(m^3\right) \quad \text{or} \quad m_{H2}\left(kg\right) < 2.61 \cdot 10^{-4}\, V\left(m^3\right)$$

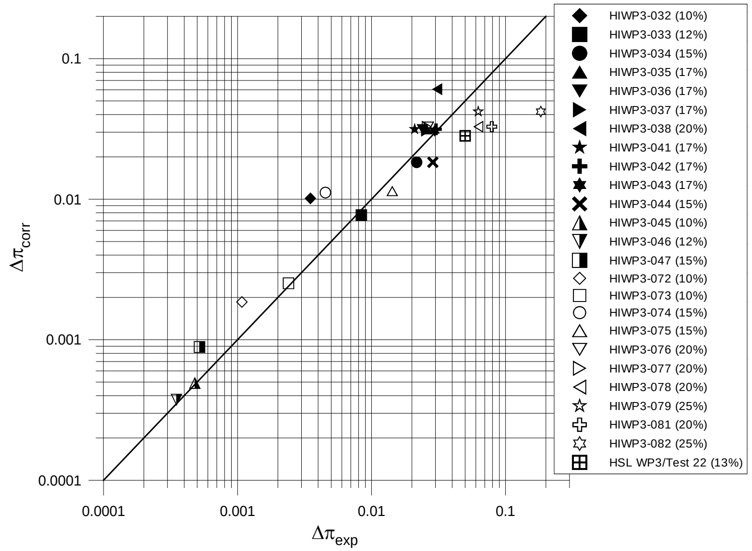
Progress: deflagrations

Localised mixture deflagration (2)

Venting correlation for localised mixtures



$$\Delta\pi = 0.018\,Br_t^{-0.92}\left(\sqrt{\frac{E_i}{2}}\cdot MIN\left\{1.0;\left[E_i^{2/3}\left(\frac{1+\left(\frac{1}{\varphi}-1\right)\frac{M_{air}}{M_f}}{1+\left(\frac{1}{\Phi\varphi}-1\right)\frac{M_{air}}{M_f}}\right)^{2/3}\right]\right\}\right)^2$$



- Applicable for vent sizing of low-strength equipment or buildings
- Only a small fraction of the non-uniform mixture with highest burning velocity (between 0.95 and 1.0 of S_u) has decisive effect on the maximum overpressure
- Model validated against 25 uniform and non-uniform mixture experiments carried out in facilities at KIT (Germany) and at HSL (UK)

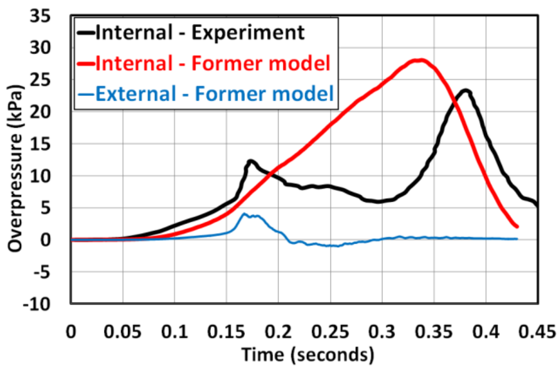
Progress: deflagrations

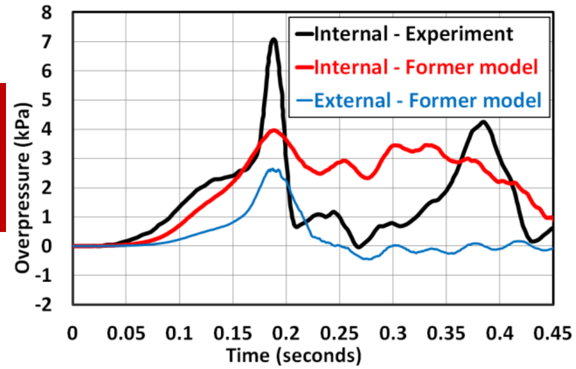
Rayleigh-Taylor instability model

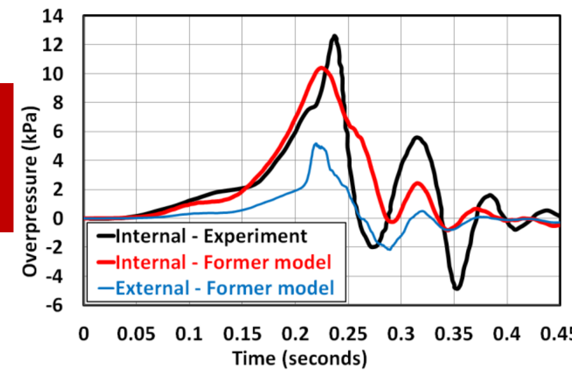
Experiment: C. Bauwens, J. Chaffee & S. Dorofeev, "Vented explosion overpressures from combustion of hydrogen and hydrocarbon mixtures," IJHE, vol.36, no. 3, pp. 2329-2336, Feb. 2011

Central ign. / 2.7m^2 vent | **Central ign. / 5.4m^2 vent** | **Back wall ign. / 5.4m^2 vent**

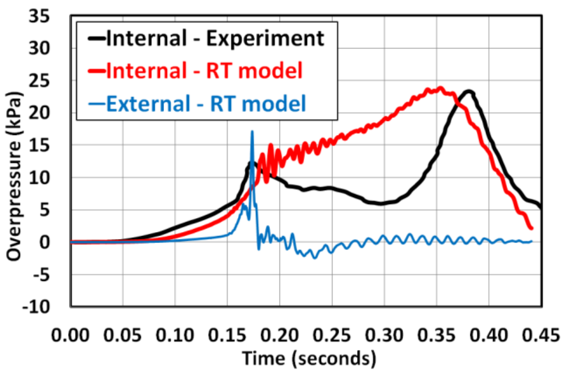
Former model results:

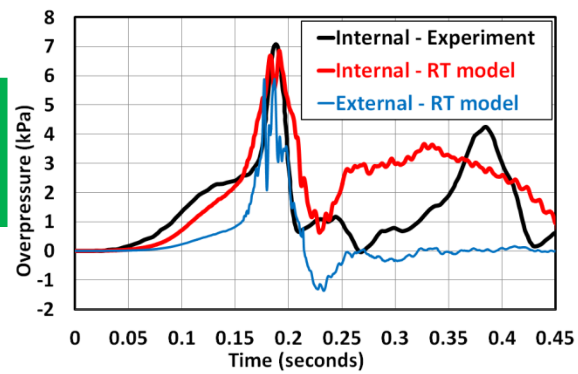


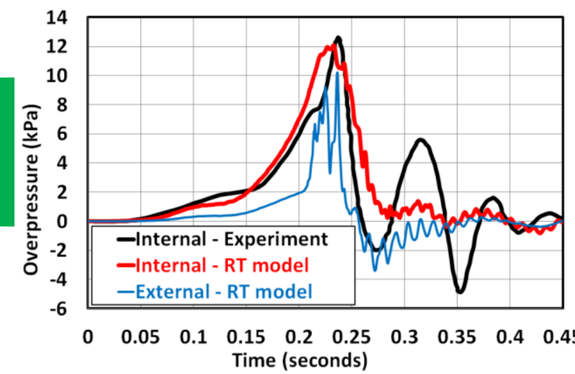




RT model results:



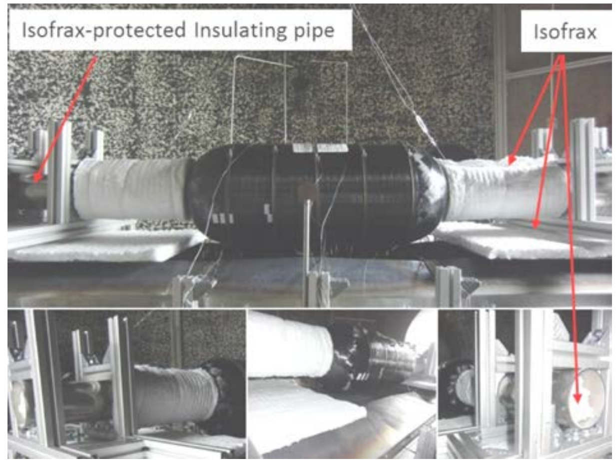




Keenan J., Makarov D., Molkov V. "Rayleigh-Taylor instability: Modelling and effect on coherent deflagrations", IJHE, V.39, No. 35, pp20467-20473, 2014

Progress: storage safety

Thermal protection and fire resistance



Exp. No	Tank condition	Tank condition	HRR, kW	Protection	Ambient gas	Filling gas	FRR
1	Bare	New	170	-	N_2	H_2	8 min
2	Bare	Used	170	-	N_2	H_2	9.7 min
3	Bare	Used	79	-	N_2	H_2	16 min
4	Protected	Used	170	Intumescent paint, 7 mm	Air	He	1 h 7 min
5	Protected	Used	170	Intumescent paint, 20 mm	Air	He	1 h 50 min
6	Protected	Used	170	Outer shell	Air	He	1 h 13 min

HRR *vs* FRR

FRR *vs* thermal protection

- KIT HyKA facility, premixed burner (Int. Access programme within H2FC project)
- Type 4, pressure loaded tanks, bare and protected, 6 completed fire tests
- Uncertainty in heat release rating (HRR) allows for discrepancy in fire resistance between test centres
- Achieved fire resistance rating (FRR) **1h 50min -** beyond the longest experimental car fire **1h 40min**

Makarov D., Kim Y., Kashkarov S., Molkov V. "Thermal Protection and Fire Resistance of High-Pressure Hydrogen Storage", Proc. of 8th ISFEH, 25-28 April 2016, Hefei, China

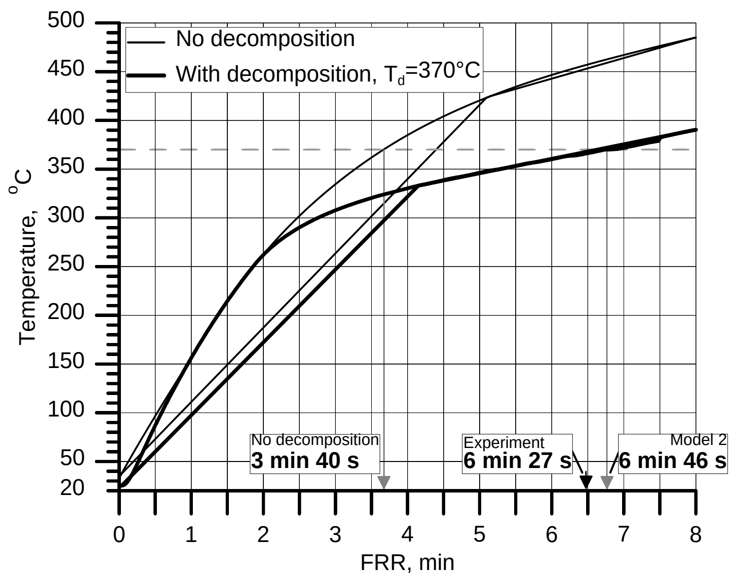
Progress: storage safety

Conjugate heat transfer to tank in fire

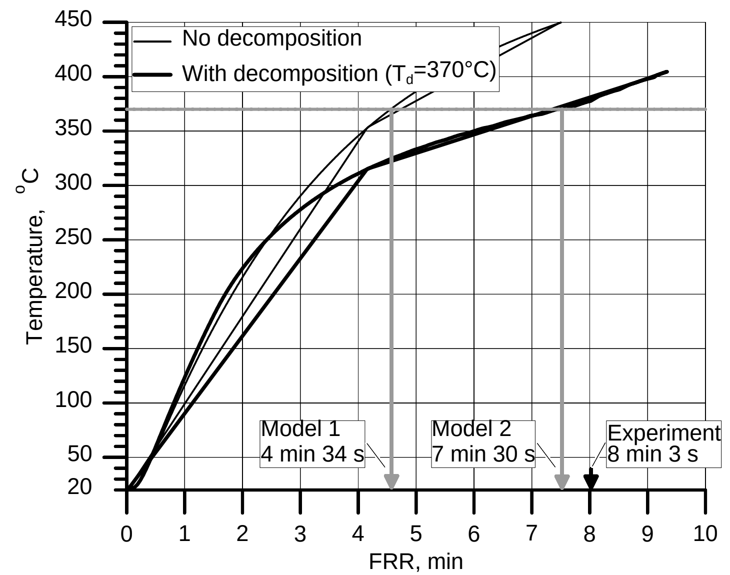
CFD model to predict tank failure

- Segregated incompressible solver, SIMPLE algorithm
- Standard $k - \varepsilon$ model with wall functions
- Eddy-Dissipation model
- Discrete Ordinates radiation model with WSGG
- Tank failure criterion based on decomposed wall thickness

Non-premixed propane burner test
(Weyandt, 2005)

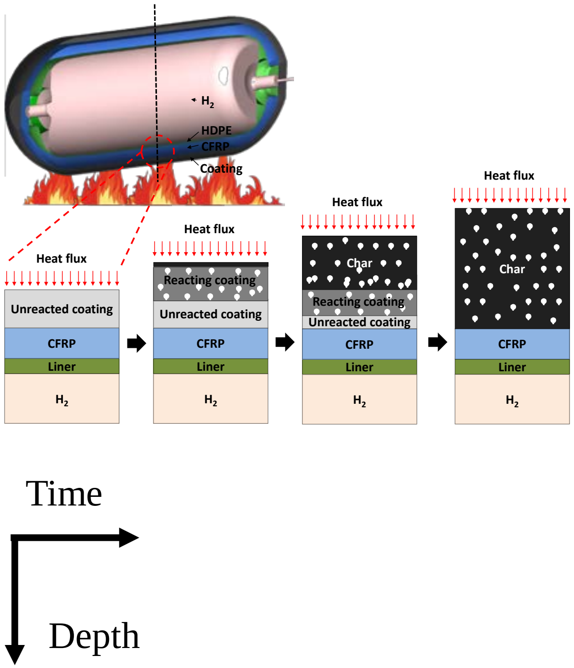


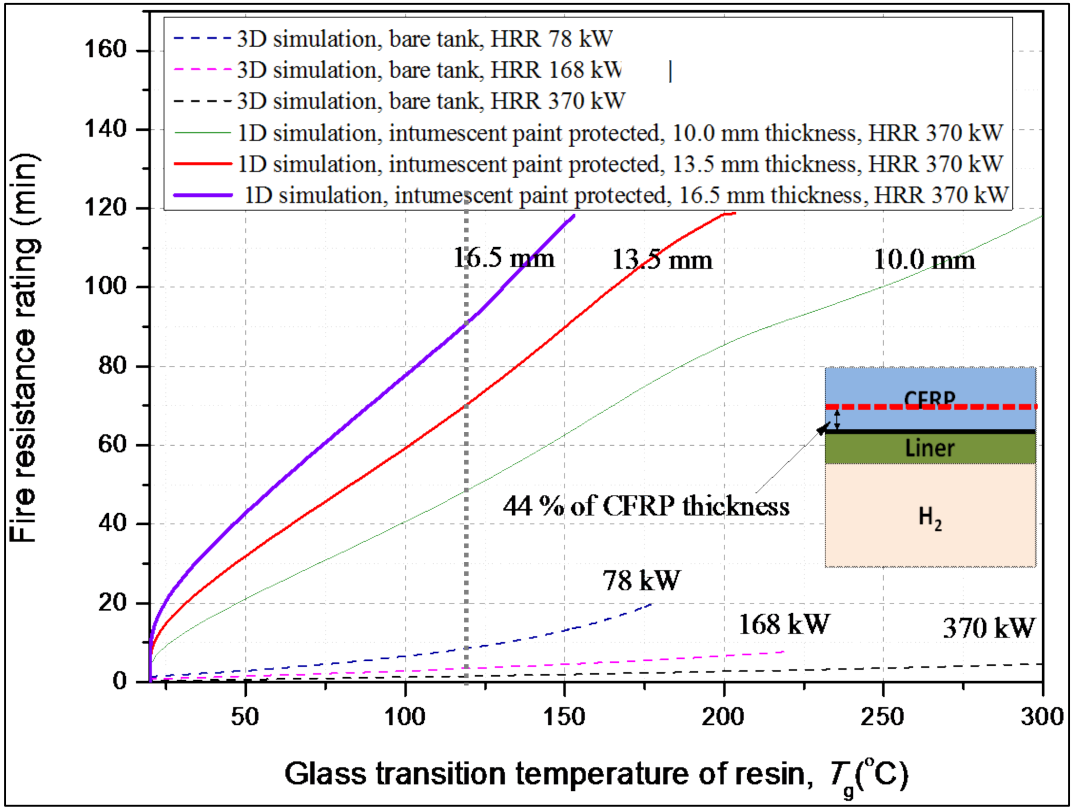
Premixed burner test
(KIT facility)



Progress: storage safety

CFD study of intumescent paint protection





Thermal protection can increase FRR by order of magnitude!

Working topics

Releases and jet fires

- Transient solution for under-expanded jet fire lift-off and blow-off
- Delayed ignition of high-pressure releases
- CGH2 and LH2 jet fire flame length and radiation
- Effect of impinging and attached jets on hazard distances

Blast waves and fireballs

- Blast wave and fireball dynamics from high-pressure tank rupture accounting real gas properties and effect of radiation effect on blast wave decay
- Thermal radiation from fireballs

Deflagrations and detonations

- Non-uniform vented deflagration (further model validation)
- DDT modelling and simulations in large industrial scales

Working topics

Storage safety

- Breakthrough explosion-free (leak-no-burst) technology for CGH2 storage in composite tanks (patent application GB1602069.5 Composite pressure vessel, 05.02.2016)
  - Following outcomes of the UK EPSRC H2FC SUPERGEN Hub and SUPERGEN Challenge projects
- Parametric study to underpin proposal for update of GTR#13 fire test protocol
  - Effect of HRR
  - Effect of burner design and type

New directions

- Update of GTR#13 fire test protocol to harmonise test procedure and eliminate test results discrepancy in different laboratories:
  - Definition of representative value of heat release rate of test fire to reflect parameters of real car fires
  - Establish requirements to “standard” burner design
- Radiation heat transfer modelling and numerical simulations to characterise hazards related to high-pressure storage and components at refuelling stations.
- Breakthrough safety technologies development and validation, e.g. exclusion of catastrophic tank rupture in a fire.

New directions

- Prevention and mitigation of blast wave in confined space such as tunnels, garages, car parks, HRS, etc.
- Time to rupture of high-pressure vessel, e.g. tube at road accident, subject to jet fire from high-pressure equipment, e.g. another tube.
- Efficiency of blast barrier designs.
- Harmful pressure and thermal effects on first responders (with protection).
- Pressure peaking phenomena for ignited releases.
- Thermal loads of indoor fires and effect of water condensation.
- Attached and impinging jets: CFD modelling and engineering correlations.
- LH2 tank rupture and rapid phase transition pressure loads.

New directions

- Liquefied hydrogen release, dispersion and ventilation, including under wind conditions.
- Combustion of cold hydrogen jets and clouds during and after LH2 release.
- Passive ventilation for multiple vents under realistic wind conditions.
- Validation experiments for: under-vehicle tank rupture, tanks of different volume and pressure, etc.

Thank you for your attention!