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Pre normative research
on the indoor use of fuel cells and hydrogen systems

Localized mixture deflagrations: the inventory limit strategy, and mitigation by venting technique

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Hydrogen inventory limitation for preventing enclosure damage

Motivation

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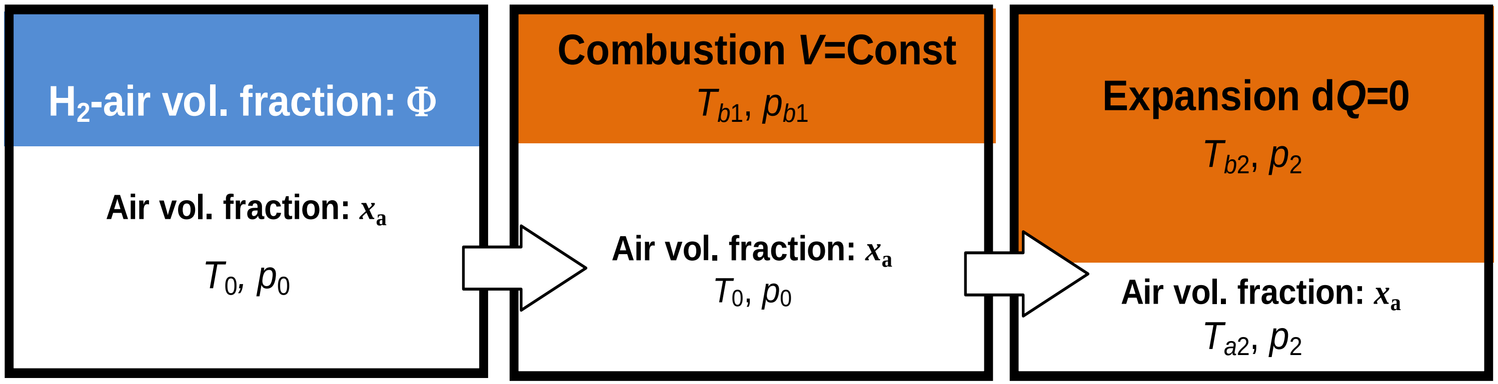
- Hydrogen inventory (stored mass) limitation is one of safety strategies for indoor use of hydrogen
- Criterion of 10 kPa deflagration overpressure (typical limit for minor damage like windows breakage, etc.) is chosen to define the upper hydrogen inventory limit in a poorly ventilated ("closed") enclosures like some warehouses, etc.
- The presented here model was applied to find hydrogen mass allowed to be released in an enclosure and combust without causing overpressures above 10 kPa

The model

- Calculation scheme: closed volume adiabatic combustion



- Final analytical solution:

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

Φ – volume fraction of H_2-air mixture in enclosure

φ - volume fraction of H_2 in H_2-air mixture

p_0 – initial pressure

p_{b1} – pressure after H_2-air mixture combustion (*V*=Const)

p_2 - pressure after burnt mixture expansion (d*Q*=0)

Validation of the model

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- Ref.: *Stamps D., et al. "Pressure rise generated by the expansion of a local gas volume in a closed vessel". Proc. R. Soc. A 465, 3627-3646, 2009* (doi:10.1098/rspa.2009.0140)
- Equivalence ratio of hydrogen-air mixture: 0.997

H2-air mixture fraction, Φ	Inert gas fraction, 1-Φ	Inert gas	Initial pressure p_0, kPa	Experimental overpressure p_{b1}, kPa	Experimental overpressure p_2, kPa	Model solution	
						p_2, kPa	error, %
0.4686	0.5314	CO2	105.5	599.7	295.7	305.2	3.18
0.8783	0.1217	CO2	109.3	632.1	491.9	555.1	12.85
0.4686	0.5314	He	105.4	598.9	335.8	326.0	-2.93
0.8783	0.1217	He	105.8	612.2	553.1	546.1	-1.26
0.4686	0.5314	N2	104.7	595.4	316.5	309.5	-2.22
0.8783	0.1217	N2	109.8	635.3	530.1	560.7	5.77

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The inventory limit

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- Parametric study:
  - → Layers with different hydrogen concentration (φ), occupying different fraction of enclosure volume (Φ) targeting (p_2-p_0)=10 kPa.

φ	Φ	$x_{H2} = \varphi \cdot \Phi$
0.04	0.0786	$3.14 \cdot 10^{-3}$
0.08	0.0474	$3.79 \cdot 10^{-3}$
0.12	0.0355	$4.26 \cdot 10^{-3}$
0.16	0.0293	$4.69 \cdot 10^{-3}$
0.20	0.0253	$5.06 \cdot 10^{-3}$

- Conclusion:
  - → The lower hydrogen mole fraction in a layer the lower mole fraction **averaged through the enclosure** (for 10 kPa overpressure)

Input to the Guidelines

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- To prevent pressure built up above 10 kPa:
  - Average hydrogen volumetric fraction in enclosure (hydrogen volumetric inventory at NTP divided by enclosure volume) should be below 0.00314, i.e. 0.3% v/v (we are not protected if H2 averaged concentration is above 0.3% by volume). This is below of LFL of 4%!
  - Otherwise (in terms of inventory and enclosure volume): $m_{H2}/V<0.261$ g/m3 (*m* – hydrogen inventory, *V* – enclosure volume). Note: LFL is 3.33 g/m3! Examples:

Enclosure volume, m^3	1	10	100	1,000	100,000
Inventory in m^3	0.00314	0.0314	0.314	3.14	314
Inventory in kg	$2.61 \cdot 10^{-4}$	$2.61 \cdot 10^{-3}$	$2.61 \cdot 10^{-2}$	0.261	26.1

- Solution is conservative (assumes no venting of deflagration

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Concluding remarks

- A model to find a maximum hydrogen inventory for use in poorly ventilated enclosures or enclosures without specially provided ventilation was developed and validated against data by Stamps et al. (2009) within HyIndoor
- Conservative solution for the hydrogen inventory limit is obtained targeting maximum overpressure 10 kPa as a safety criterion (0.261 g/m3)
- Where the inventory is larger than the specified limit, the use of other mitigation techniques should be considered (natural/forced ventilation to exclude flammable mixture formation, deflagration venting, etc.)

Mitigation of localized mixture deflagrations by venting

Motivation

- Available vent sizing methodologies are applicable to uniform fuel-air mixtures occupying the whole enclosure only
- Deflagration of non-uniform or layered mixtures can generate overpressure above that for uniform mixture deflagration (the same amount of hydrogen)
- Maximum overpressure depends strongly on portion of mixture with largest hydrogen concentration
- HyIndoor experimental data were used for validation of previously developed theory (*Molkov, DSc thesis, 1996*)

Layered mixture

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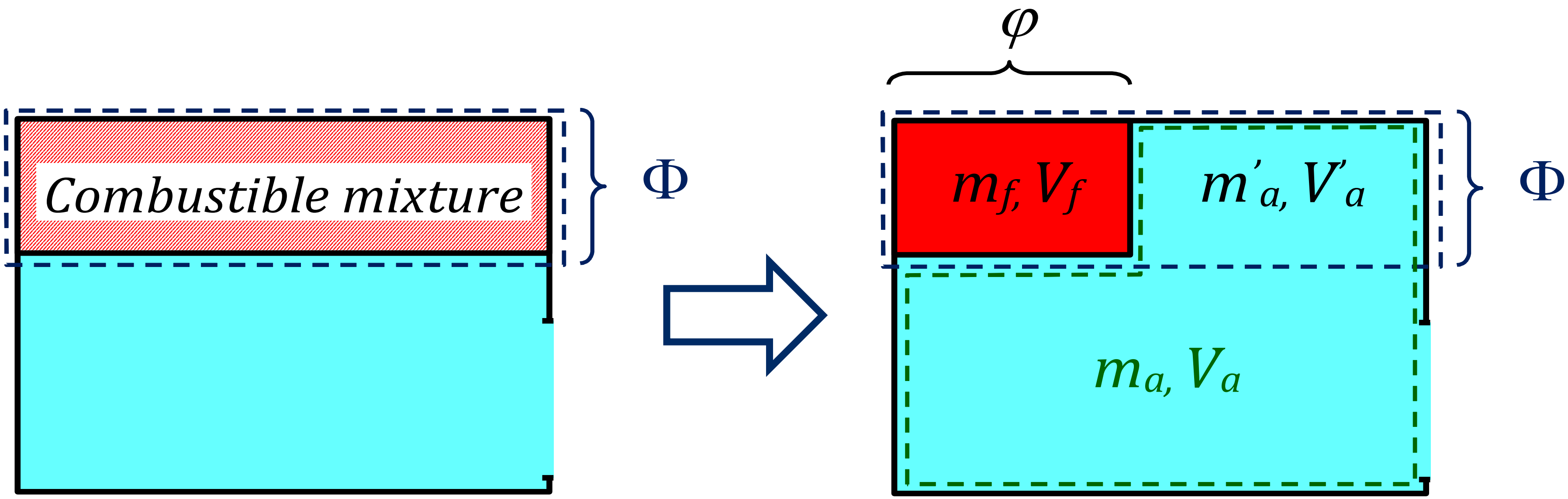
Calculation scheme



Initial volume fraction of unburnt mixture $\Phi = w_{ui} = \left(V_{fi} + V'_{ai}\right)/\left(V_{fi} + V_{ai}\right)$

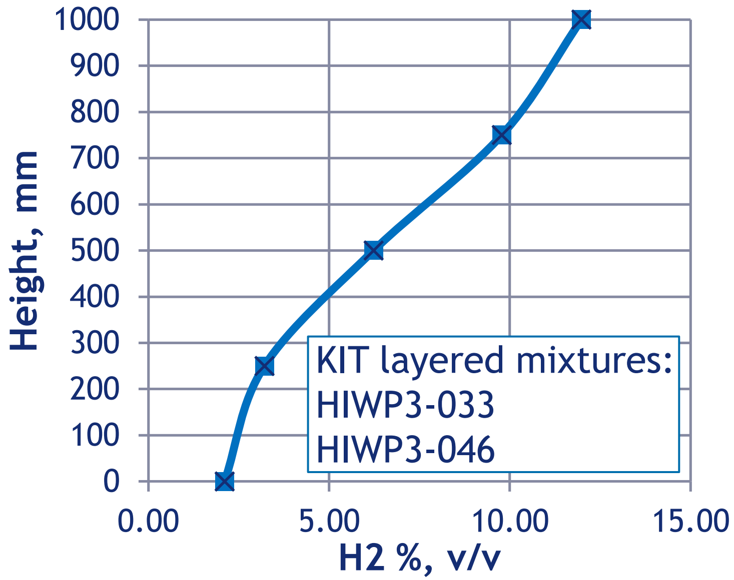
Volume fraction of fuel in combustible mixture $\varphi = V_f / \left(V_f + V'_a\right)$

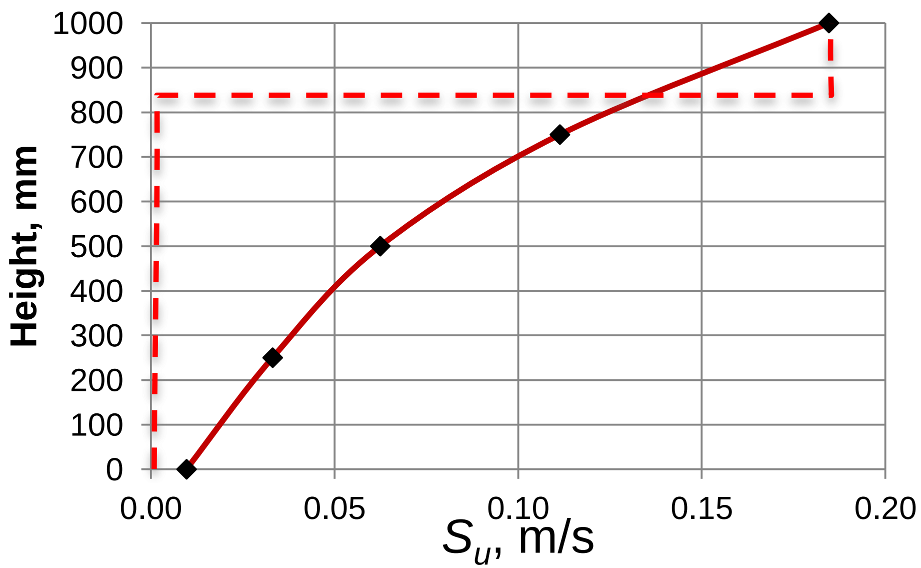
Volume fraction of unburnt mixture $\omega_u = \left(V_f + V'_a\right)/V$

Mass fraction of unburnt fuel-air mixture $n_u = \left(m_f + m'_a\right)/\left(m_f + m_a\right)$

Methodology (1/2)

- Calculate dimensionless reduced explosion overpressure for the enclosure $\Delta\pi_r = \left(p_{\max} - p_i\right)/p_i$
- Determine distribution of burning velocity $S_{u0}(X_{H2})$
- Determine unburnt mixture Φ (it is counted as mixture in the range of burning velocity: $(0.7 \div 1.0) \cdot S_u$





Φ=0.19 as a fraction of mixture within range $(0.7 \div 1.0) \cdot S_u$

Methodology (2/2)

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- Determine unburnt mixture properties: E_i, γ, S_{ui}, m_0, c_{ui}, R_0
- Find Br_t from the correlation equation (see graph below):

$$Br_t = \left(4\Delta\pi_r\right)^{1.06} \left(E_i/\gamma\right)^{1/2} E_i^{2/3} \Phi^{2/3} / \sqrt{2}$$

- From calculation of wrinkling factors Ξ_K, Ξ_{FR}, Ξ_{lp}, $\Xi_{u'}$, Ξ_{AR} find out the DOI number:

$$\chi/\mu = \Xi_K \cdot \Xi_{FR} \cdot \Xi_{lp} \cdot \Xi_{u'} \cdot \Xi_{AR}$$

- Find Bradley number:

$$Br = \sqrt[3]{36\pi_0} \cdot \chi/\mu \cdot Br_t / \sqrt{E_i/\gamma_u}$$

- Find vent area:

$$F = Br \cdot V^{2/3} \cdot S_{ui} \cdot \left(E_i - 1\right)/c_{ui}$$

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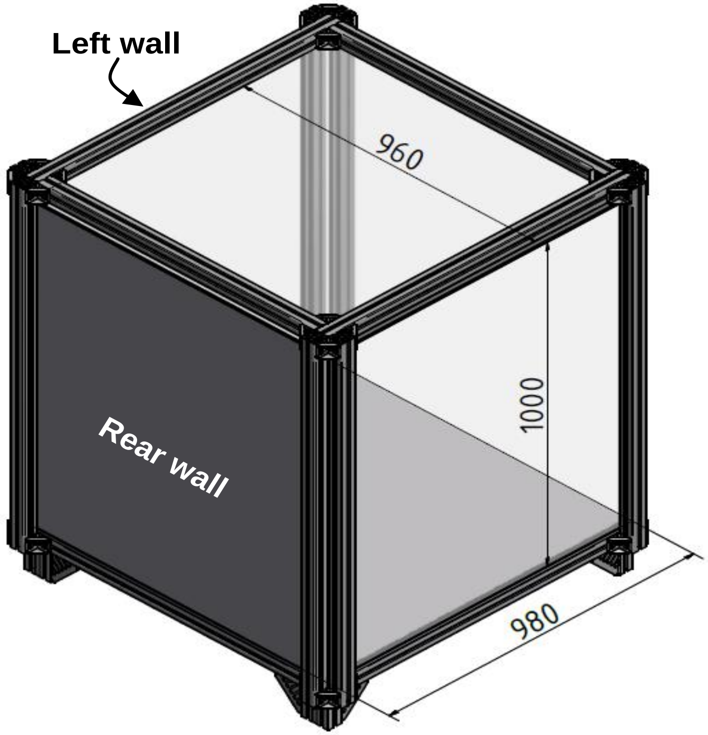
Experimental facilities

KIT

- LxHxW=0.98x1.00x0.96 m
- Vents: 0.10x0.10 m to 0.50x0.50 m
- Ignition:
  - rear, at the rear wall centre
  - rear, under top plate



HSL

- LxHxW=5.0x2.5x2.5 m
- Vent: 0.448 m^2
- Ignition:
  - rear, at the rear wall centre

Uniform layer results

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	Experiment				Correlation								
	Φ, %	φ, %	Vent area, m^2	$p_{red.exp}$	S_{ui}, m/s	E_i	C_{ui}, m/s	R_o, m	Ξ_K	Ξ_{LP}	Ξ_{FR}	χ/μ	$p_{red.corr}$
HIWP3-072	25	10	0.5×0.5	0.00108	0.111	3.5	361	0.55	1.3	2.31	1.038	3.87	0.00104
HIWP3-073	50	10	0.5×0.5	0.00240	0.111	3.5	361	0.55	1.3	2.31	1.038	3.87	0.00193
HIWP3-074	25	15	0.5×0.5	0.00452	0.346	4.56	371	0.89	1.53	2.02	1.0	3.83	0.00834
HIWP3-075	50	15	0.5×0.5	0.0143	0.346	4.56	371	0.89	1.53	2.02	1.0	3.83	0.0157
HIWP3-076	25	20	0.5×0.5	0.0266	0.830	5.52	381	1.2	1.65	1.75	1.0	3.58	0.0357
HIWP3-077	25	20	0.5×0.5	0.0258	0.830	5.52	381	1.2	1.65	1.75	1.0	3.58	0.0357
HIWP3-078	50	20	0.5×0.5	0.0627	0.830	5.52	381	1.2	1.65	1.75	1.0	3.58	0.0679
HIWP3-079	25	25	0.5×0.5	0.0626	1.502	6.36	393	1.2	1.53	1.52	1.0	2.89	0.0759
HIWP3-081	50	20	0.5×0.5	0.0790	0.830	5.52	381	1.2	1.65	1.75	1.0	3.58	0.0679
HIWP3-082	50	25	0.5×0.5	0.183	1.502	6.36	393	1.2	1.53	1.52	1.0	2.89	0.146

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Gradient layer results

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Experiment						Correlation								
	H_2,vol	Φ, %	φ, %	Vent area, m^2	$P_{red.exp}$	S_{ui}, m/s	E_i	C_{ui}, m/s	R_o, m	Ξ_K	Ξ_{LP}	Ξ_{FR}	χ/μ	$P_{red.corr}$
HIWP3-032	10-5%	44.7	10.00	0.1×0.1	0.0035	0.117	3.50	361	0.55	1.08	2.31	1.04	3.23	0.0045
HIWP3-033	12-2%	18.9	11.98	0.1×0.1	0.0084	0.185	3.94	365	0.69	1.27	2.19	1.00	3.46	0.0055
HIWP3-034	15-4%	19.3	14.95	0.1×0.1	0.0217	0.358	4.55	371	0.89	1.54	2.02	1.00	3.85	0.0169
HIWP3-035	17-4%	17.1	16.98	0.1×0.1	0.0258	0.530	4.95	375	1.02	1.71	1.91	1.00	4.05	0.0293
HIWP3-036	17-4%	17.1	16.98	0.1×0.1	0.0240	0.530	4.95	375	1.02	1.71	1.91	1.00	4.05	0.0293
HIWP3-037	17-6%	16.9	16.94	0.1×0.1	0.0255	0.527	4.94	375	1.02	1.71	1.91	1.00	4.05	0.0287
HIWP3-038	20-4%	16.2	20.00	0.1×0.1	0.0309	0.862	5.52	381	1.20	1.96	1.75	1.00	4.25	0.0609
HIWP3-041	17-4%	17.1	16.98	0.1×0.1	0.0210	0.530	4.95	375	1.02	1.71	1.91	1.00	4.05	0.0293
HIWP3-042	17-4%	17.1	16.98	0.1×0.1	0.0303	0.530	4.95	375	1.02	1.71	1.91	1.00	4.05	0.0293
HIWP3-043	17-6%	16.9	16.94	0.1×0.1	0.0296	0.527	4.94	375	1.02	1.71	1.91	1.00	4.05	0.0287
HIWP3-044	15-4%	19.3	14.95	0.1×0.1	0.0287	0.358	4.55	371	0.89	1.54	2.02	1.00	3.85	0.0169
HIWP3-045	10-5%	44.7	10.00	0.5×0.5	0.0005	0.117	3.50	361	0.55	1.08	2.31	1.04	3.23	0.0001
HIWP3-046	12-2%	18.9	11.98	0.5×0.5	0.0004	0.185	3.94	365	0.69	1.27	2.19	1.00	3.46	0.0002
HIWP3-047	15-4%	19.3	14.95	0.5×0.5	0.0005	0.358	4.55	371	0.89	1.54	2.02	1.00	3.85	0.0006
HSL Test 22	23 – 0%	28.8	23.2	0.448	0.0600	1.29	6.07	388	1.20	2.93	1.60	1.17	7.17	0.0517

The correlation

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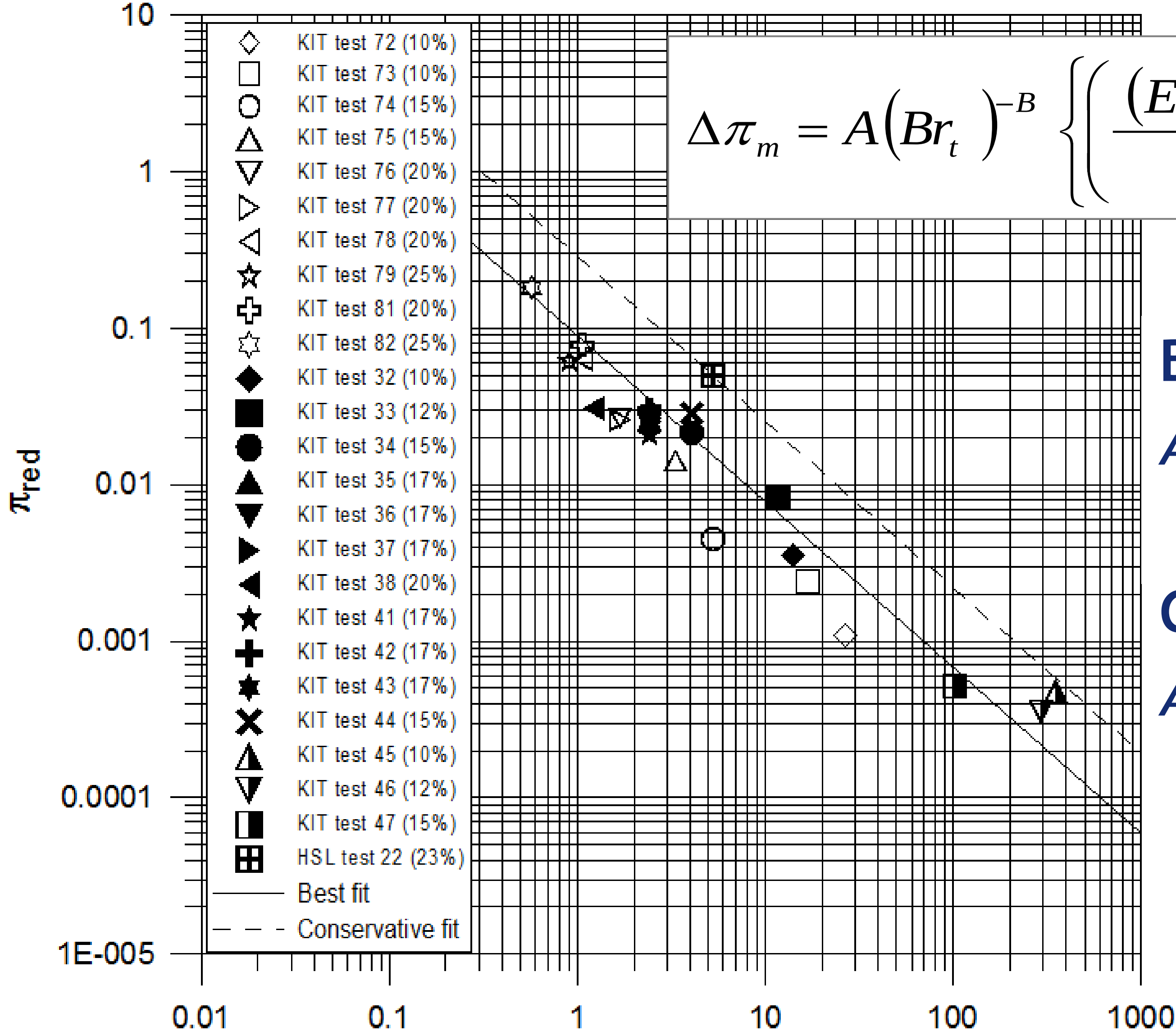
$$\Delta\pi_m = A\left(Br_t\right)^{-B}\left\{\left(\frac{\left(E_i/\gamma\right)^{1/2}E_i^{2/3}}{\sqrt{2}}\right)\Phi^{2/3}\right\}^{B}$$



$$\frac{Br_t\sqrt{2}}{(E/\gamma)^{1/2}(E)^{2/3}\Phi^{2/3}}$$

Best fit:

A=0.09, *B*=1.06

Conservative fit:

A=0.29, *B*=1.06

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Concluding remarks

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- The analytical model for maximum overpressure in a vented deflagration of localised fuel-air mixture is described in detail in HyIndoor deliverable D3.4
- The theory-based correlation was developed and validated against experimental data by KIT and HSL
- Best fit and conservative correlations are included in the Guidelines

Acknowledgements

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