NTNU
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Modelling of accident scenarios from hydrogen transport and use

RAMS PhD seminar

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28.04.2022

Content

Hydrogen properties

Property	Value
Gravimetric energy density (MJ/kg) [3]	119.96
Combustion products	Water, NOx (avoidable)
Toxic	No
Density at NTP (kg/m^3) [4]	0.0883
Minimum ignition energy (mJ) [5]	0.017
Flammability range in air (%vol) [6]	4 ÷ 75
Flame visibility	Scarce
Colour and/or odour	None
Molecule diameter (pm)	120

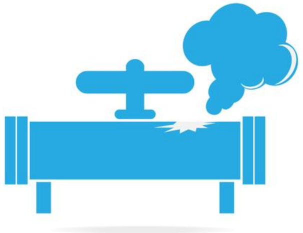
Volatile (safety)

Storage issue

Highly flammable

Difficult to detect

Difficult to contain



Liquid hydrogen hazards

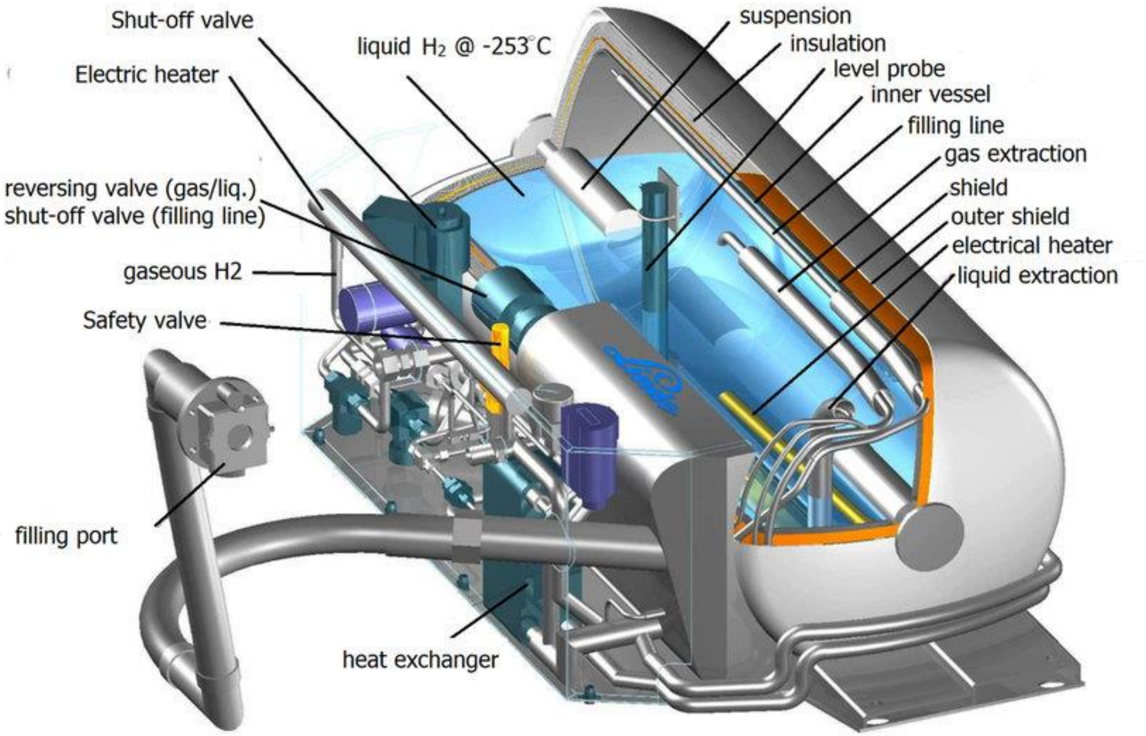
Liquid hydrogen (LH2) properties:

- ✓ Density: 70.9 kg/m3
- ✓ Normal boiling temperature: 20.7 K (-253°C)

LH2 tanks:

- ✓ Double-walled vacuum insulated
- ✓ Operative pressure: ~1 bar
- ✓ Maximum allowable pressure: 10 bar

<u>Consequences of LOC: BLEVE, RPT</u>



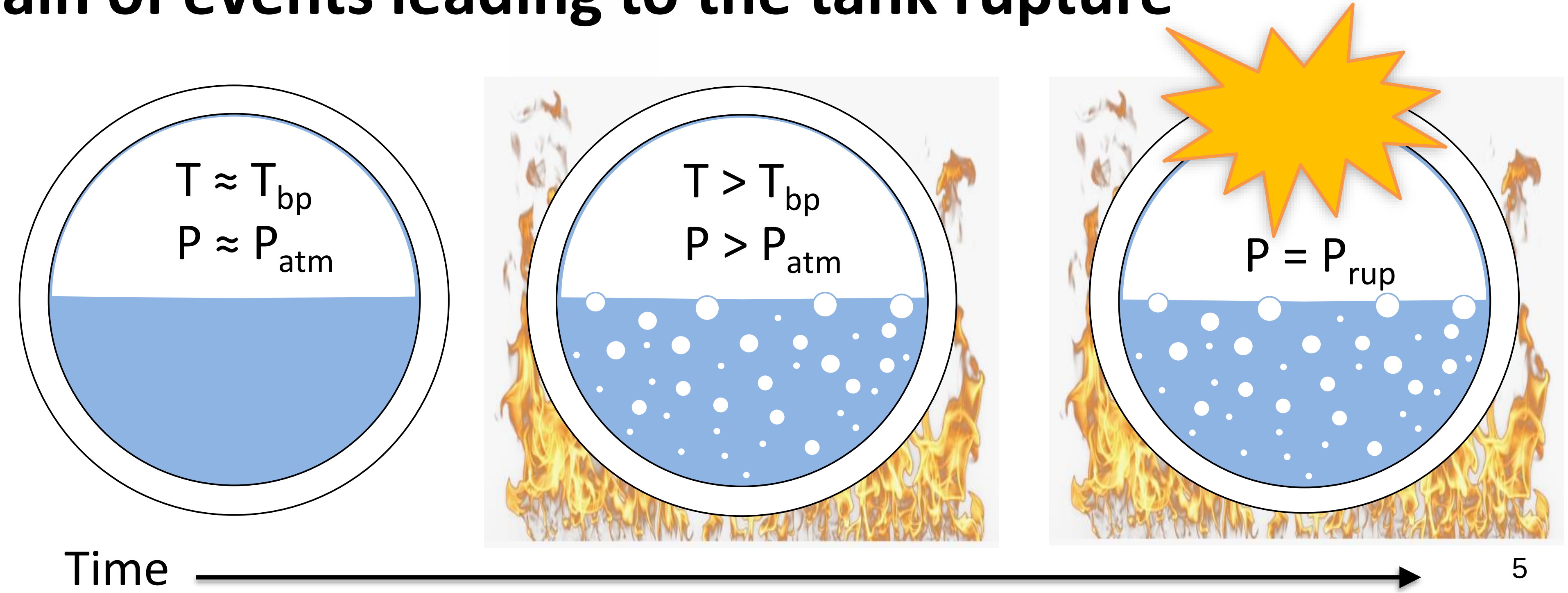
LH2 automotive tank (source: BMW)

Boiling Liquid Expanding Vapour Explosion

BLEVE is a physical explosion might result from the catastrophic rupture of a tank containing a superheated liquid due to the rapid depressurization

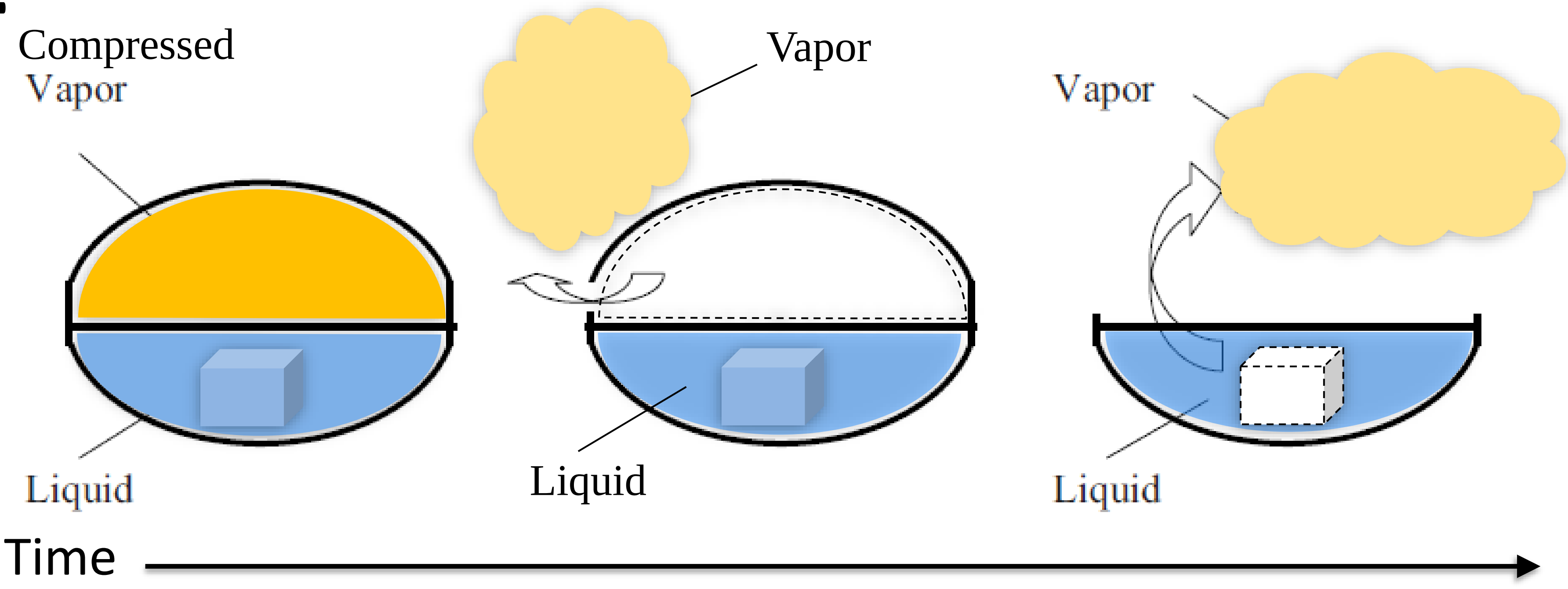
Chain of events leading to the tank rupture

Valid for cryogenic substances



LH2 hazards

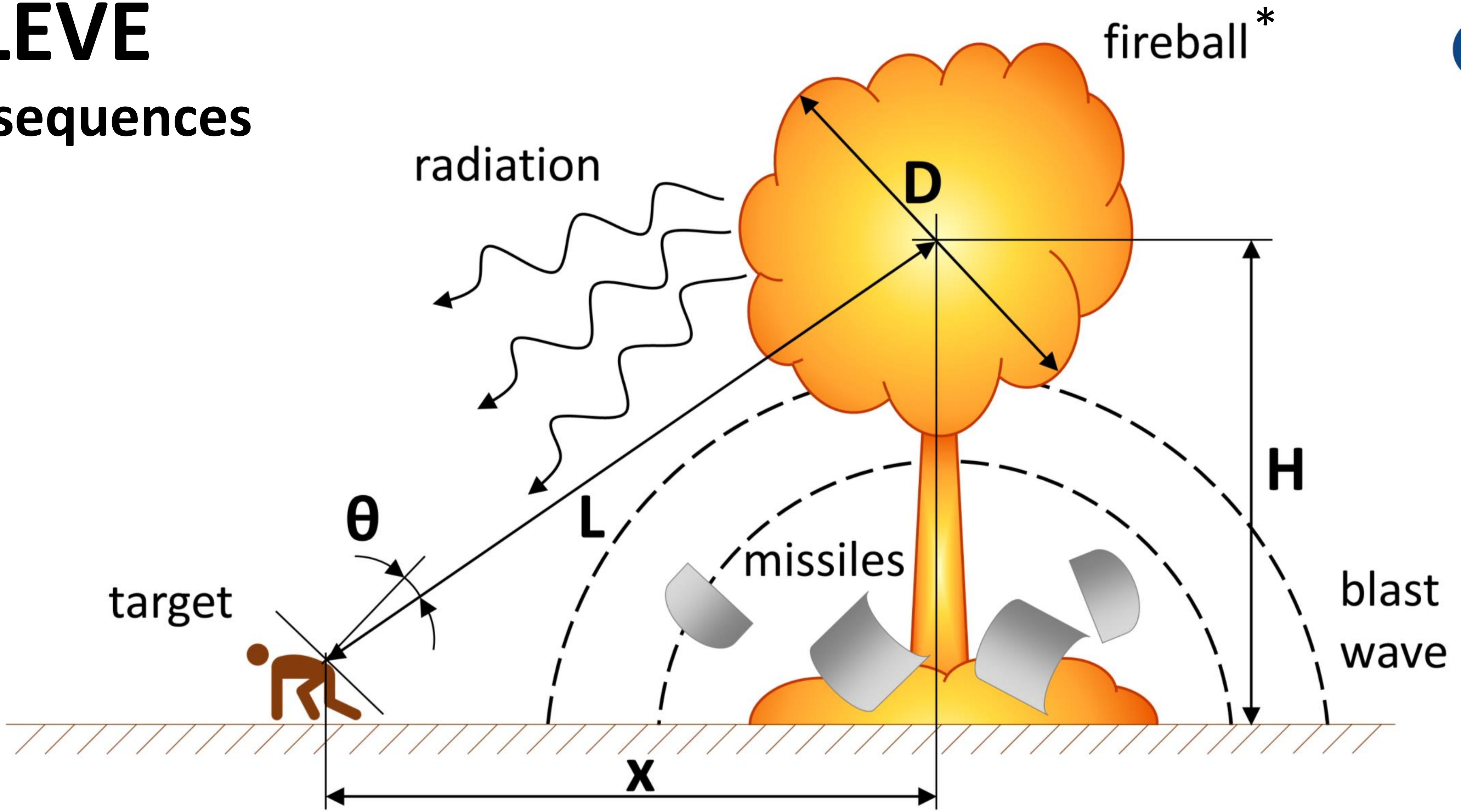
BLEVE



P	$P_o = 101.3\ kN\ m^{-2}$	$P_o = 101.3\ kN\ m^{-2}$
$T = T_s(P)$	T	$T_o = T_s(P_o)$
$h_l = h_l(T)$	$h_l(T, P_o) \approx h_l(T)$	$h_{lo} = h_{lo}(T_o)$
$h_g = h_g(T)$	**metastable/unstable**	$h_{go} = h_{go}(T_o)$

Hot liquid undergoing sudden depressurization in a tank
(adapted from [Casal, 2008])

BLEVE
Consequences



*Fireball if substance is flammable and ignition source is present

LH2 BLEVE

Two LH_2 BLEVE occurred in the past:

1974: an LH_2 tank of 9,000 gal (34 m^3) underwent a BLEVE after the tank and its safety devices (PRV) were sprayed with water due to a near by fire [30].

1986: space shuttle “Challenger” disaster. Hot gases from the main rocket impinged the LH_2 and LOX tanks provoking a BLEVE.

[Feldman et al., “1974 LHY Tank Failure”, SAF75U002 RRS . Air Products internal report (1975)

Source: hystory.com

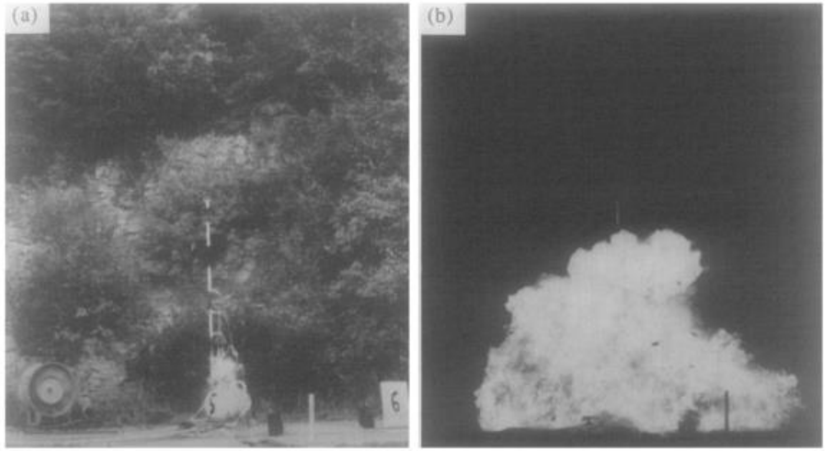
LH2 hazards

BMW safety programme

SH_2IFT LH_2 experiment has been delayed, therefore the results from the BMW tests were exploited.

Figure 11: Bonfire test of a liquid hydrogen fuel tank (Source: BAM)

Fire tests: double walled vessel filled at 50% fully engulfed in propane fire.



Development of a fireball. (a) Ignition; (b) 250 ms after ignition

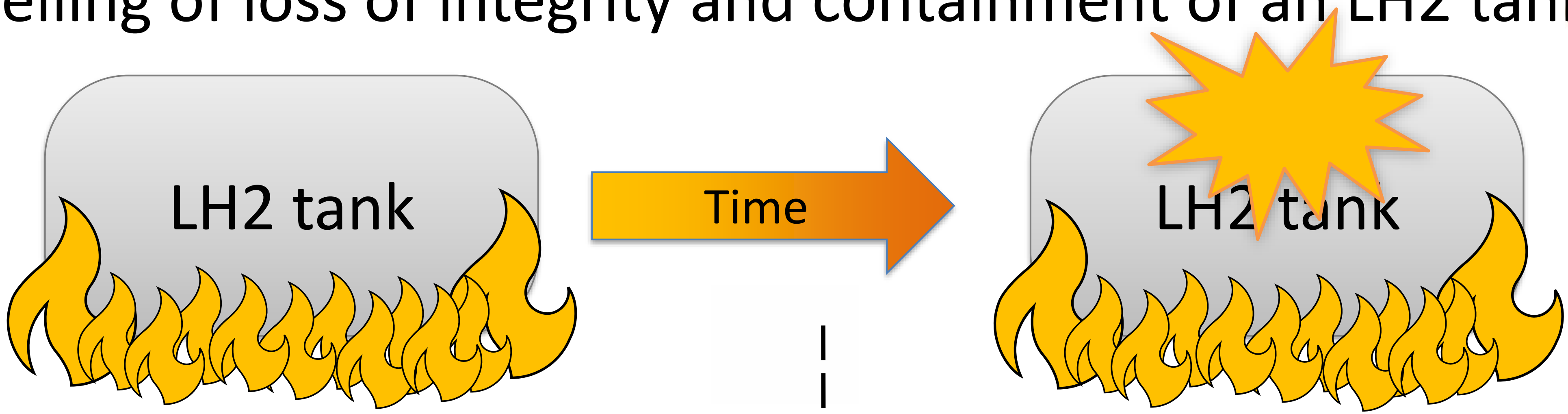
Bursting tank scenario test: ten vessels (0.120 m^3) filled with different amount of LH2 (1.8 ÷ 5.4 kg) were wrecked by means of cutting charges.

A 7 Series BMW with hydrogen IC engine and LH_2 storage

[Pehr K. Aspects of safety and acceptance of LH2 tank systems in passenger cars. Int J Hydrogen Energy 1996;21:387–95]

Consequence analysis (CA)

Modelling of loss of integrity and containment of an LH2 tank



Fire test:

- Pressure build up and temperature gradient in LH2 tank

How:

1. Lumped models
2. Numerical models (CFD)

Catastrophic rupture (BLEVE):

- Pressure wave
- Fragments
- Fireball

How:

1. Engineering tools
2. Numerical models (CFD)

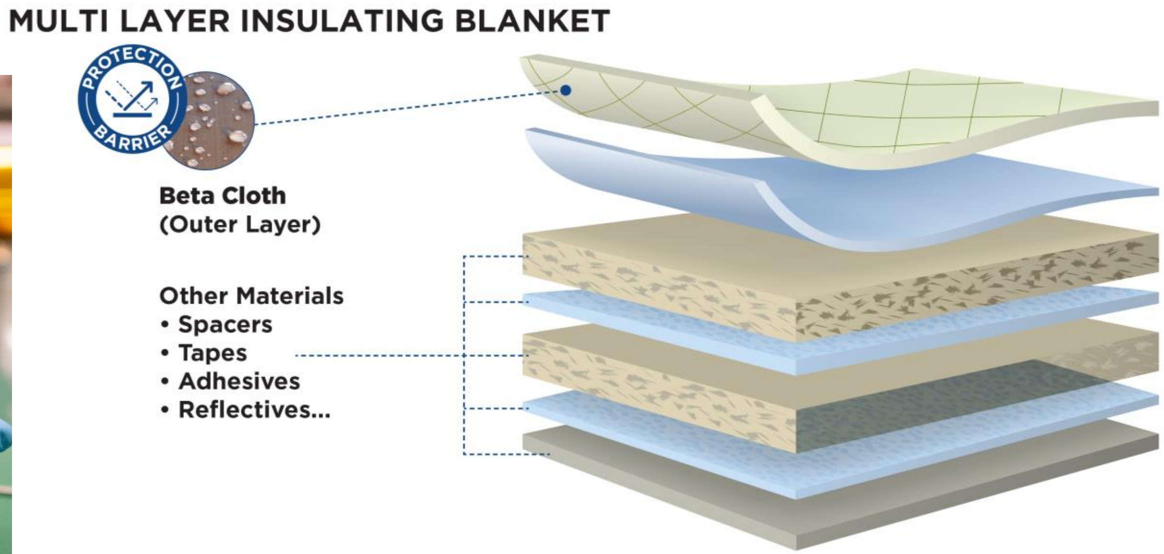
Fire test modelling

Two approaches were selected to estimate the behaviour of an LH2 tank during an accident scenario (e.g. fire):

1. Lumped model (differential equation system)
2. Computational Fluid Dynamics (CFD)

<u>Focus</u>: LH2 tank with multi-layer vacuum insulation (MLVI)


Credit: ESA-SJM Photography



Source: chemfab.com

Fire test

Lumped model - Methodology

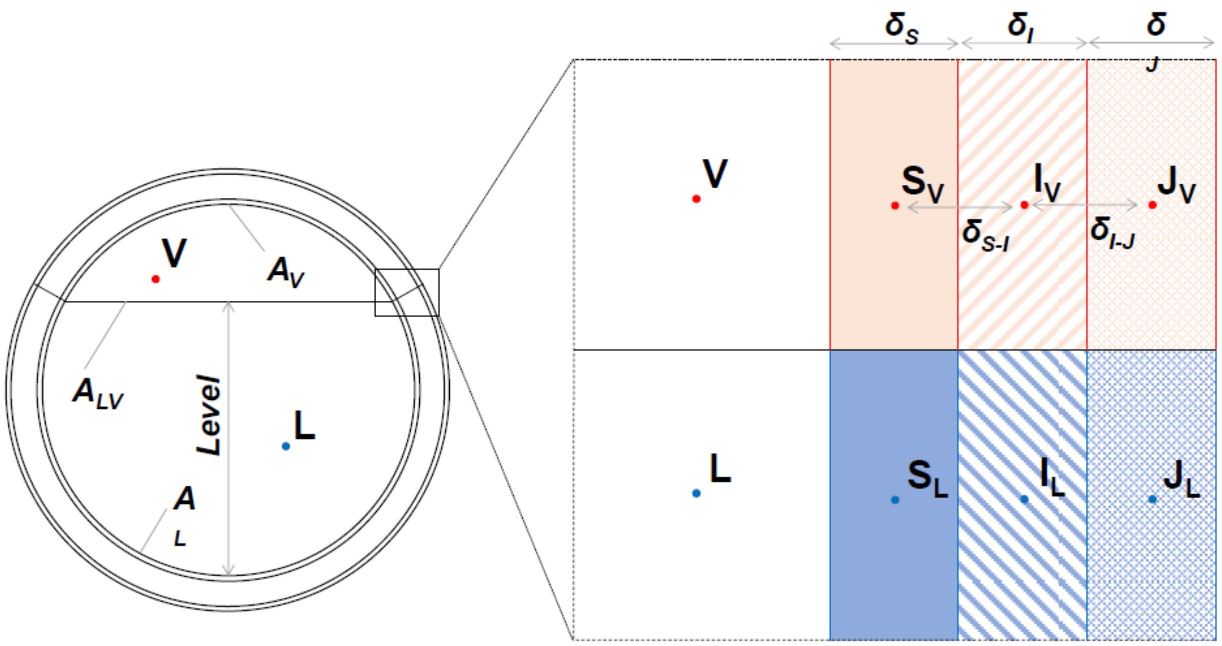


Figure 1: Schematization of thermal nodes discretization. L = liquid phase, V = vapour phase, S = shell, I = insulant, J = jacket, A_L = liquid wetted area, A_V = vapour wetted area, A_{LV} = liquid-vapour interface area.

Table 1: Thermal and mass balances for the nodes depicted in Figure 1.

Node	Variable	Equation	Eq.
L	T_L	$m_L cp_L \frac{dT_L}{dt} = A_L h_L (T_{SL} - T_L) + A_{LV} h_{LV} (T_V - T_L) + q_R + m_C(\hat{H}_V(T_V) - \hat{H}_L(T_L)) - m_E(\hat{H}_V(T_L) - \hat{H}_L(T_L))$	(1)
	m_L	$\frac{dm_L}{dt} = m_C - m_E$	(2)
V	T_V	$m_V cv_V \frac{dT_V}{dt} = A_V h_V (T_{SV} - T_V) - A_{LV} h_{LV} (T_V - T_L) - m_E \left(\hat{H}_V(T_L) - \hat{H}_V(T_L)\right) + \frac{RT_V}{M}\frac{dm_V}{dt}$	(3)
	m_V	$\frac{dm_V}{dt} = -m_C + m_E - m_{PSV}$	(4)
S_L	T_{SL}	$\delta_S \rho_{SL} cp_{SL} \frac{dT_{SL}}{dt} = -h_L(T_{SL} - T_L) + \frac{k_{S-I}}{\delta_{S-I}}(T_{IL} - T_{SL})$	(5)
S_V	T_{SV}	$\delta_S \rho_{SV} cp_{SV} \frac{dT_{SV}}{dt} = -h_V(T_{SV} - T_V) - q_R + \frac{k_{S-I}}{\delta_{S-I}}(T_{IV} - T_{SV})$	(6)
I_L	T_{IL}	$\delta_I \rho_{IL} cp_{IL} \frac{dT_{IL}}{dt} = -\frac{k_{S-I}}{\delta_{S-I}}(T_{IL} - T_{SL}) + \frac{k_{I-J}}{\delta_{I-J}}(T_{JL} - T_{IL})$	(7)
I_V	T_{IV}	$\delta_I \rho_{IV} cp_{IV} \frac{dT_{IV}}{dt} = -\frac{k_{S-I}}{\delta_{S-I}}(T_{IV} - T_{SV}) + \frac{k_{I-J}}{\delta_{I-J}}(T_{JV} - T_{IV})$	(8)
J_L	T_{JL}	$\delta_J \rho_{JL} cp_{JL} \frac{dT_{JL}}{dt} = -\frac{k_{I-J}}{\delta_{I-J}}(T_{JL} - T_{IL}) + A_L q_{FIRE}$	(9)
J_V	T_{JV}	$\delta_J \rho_{JV} cp_{JV} \frac{dT_{JV}}{dt} = -\frac{k_{I-J}}{\delta_{I-J}}(T_{JV} - T_{IV}) + A_V q_{FIRE}$	(10)
-	P	$\frac{dp}{dt} = \frac{\rho_V}{m_V}\left(\frac{P}{\rho_L}\frac{dm_L}{dt} + \frac{RT_V}{M}\frac{dm_V}{dt} + \frac{Rm_V}{M}\frac{dT_V}{dt}\right)$	(11)
-	Level	$\frac{dLevel}{dt} = \frac{1}{\rho_L}\left(\frac{dV_L}{dLevel}\right)^{-1}\frac{dm_L}{dt}$	(12)

T = temperature, m = mass, P = pressure, V_L = liquid volume, cp = specific heat capacity at constant pressure, cv = specific heat capacity at constant volume, h = convective heat transfer coefficient, $\hat{H}$ = specific enthalpy, R = gas constant, M = molecular weight, m_E = evaporation rate, m_C = condensation rate, m_{PSV} = PSV discharging rate, ρ = density, δ = thickness, k = thermal conductivity, q = heat flux

[Scarponi GE, Landucci G, Ovidi F, Cozzani V. Lumped Model for the Assessment of the Thermal and Mechanical Response of LNG Tanks Exposed to Fire. Chem Eng Trans 2016;53:307–12]

Lumped model - Assumptions

Known: tank volume (0.120 m^3), insulation thickness (35 mm)

- PRV diameter (ISO 21013-3:2016): 9.6 mm
- MLVI thermal conductivity with the Barron and Nellis (2016) procedure
- Tank dimensions:
  - diameter: 460 mm
  - length: 722 mm

[Pehr, K., 1996. Experimental examinations on the worst-case behaviour of LH2/LNG tanks for passenger cars, in: Proceedings of the 11th World Hydrogen Energy Conference, Stuttgart 23–28 June 1996. Stuttgart, pp. 2169–87]

Fire test

Lumped model - Assumptions

Initial conditions

Parameter	Units	Value
Tank filling degree	%	55
Tank pressure	bar	1.06
PRV pressure open	bar	4.68
PRV pressure close	bar	4.14
Ambient temperature	K	275
Flame temperature	K	1193
LH_2 temperature	K	20.3
H_2 temperature	K	20.3

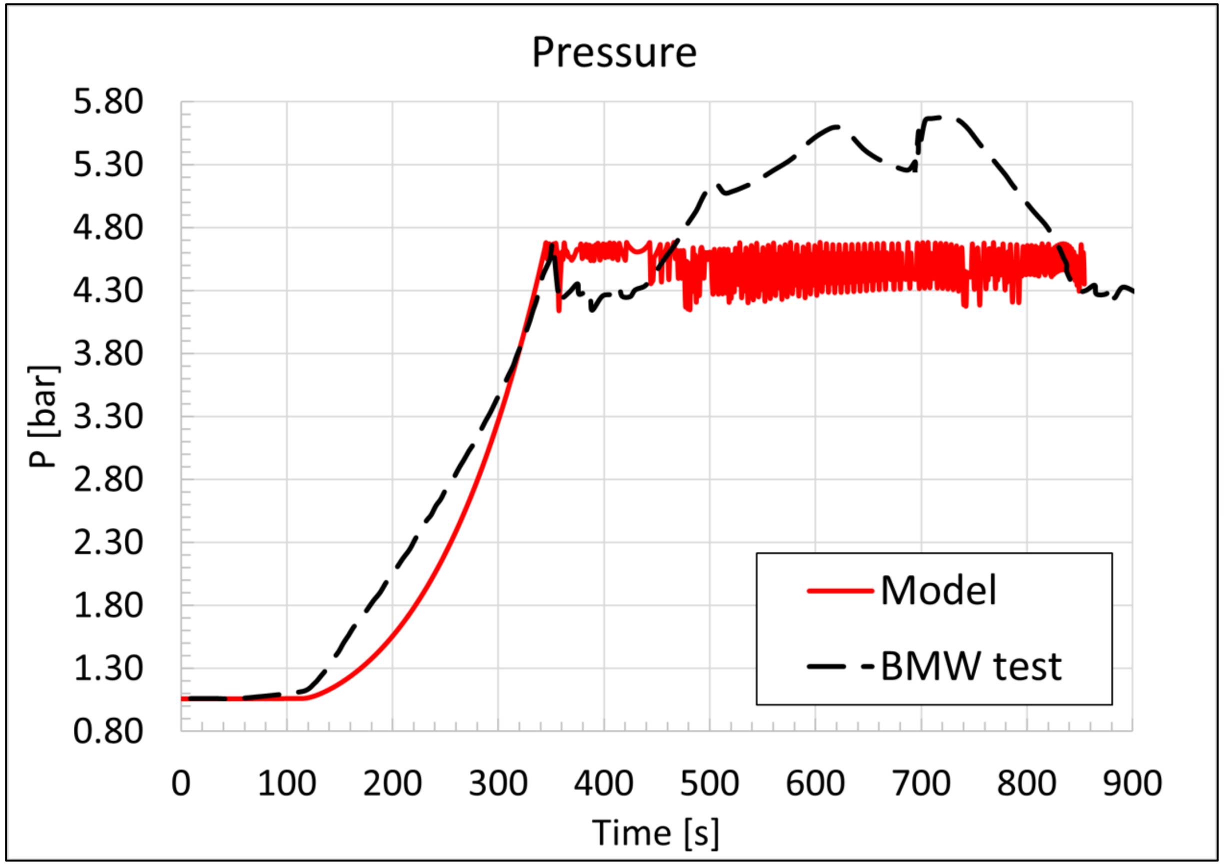
Material properties

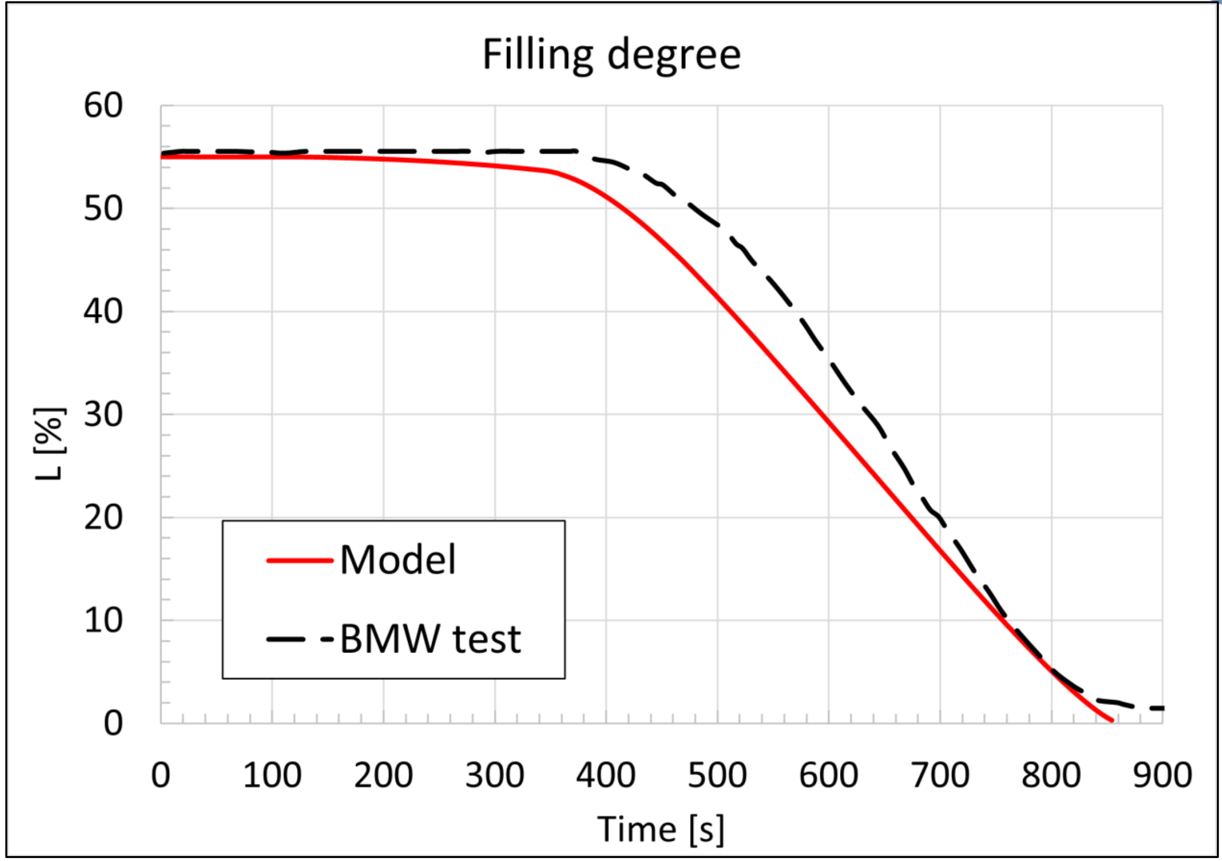
Material	Property	Units	Value
5083 Al alloy (ISO, 2014) (NIST, 2021a)	Density	$kg\ m^{-3}$	2,660
	Heat capacity	$J\ kg^{-1}\ K^{-1}$	897
	Thermal conductivity	$W\ m^{-1}\ K^{-1}$	120
	Yield strength	MPa	125
	Emissivity	-	0.9
MLVI	Density	$kg\ m^{-3}$	64*
	Heat capacity	$J\ kg^{-1}\ K^{-1}$	838*
	Thermal conductivity	$W\ m^{-1}\ K^{-1}$	0.0015*
AISI 304 (NIST, 2021b)	Density	$kg\ m^{-3}$	7,800
	Heat capacity	$J\ kg^{-1}\ K^{-1}$	490
	Thermal conductivity	$W\ m^{-1}\ K^{-1}$	16
	Yield strength	MPa	-
	Emissivity	-	0.9

At t=115 s, changed to 0.110 $W\ m^{-1}\ K^{-1}$

Fire test

Lumped model - Results

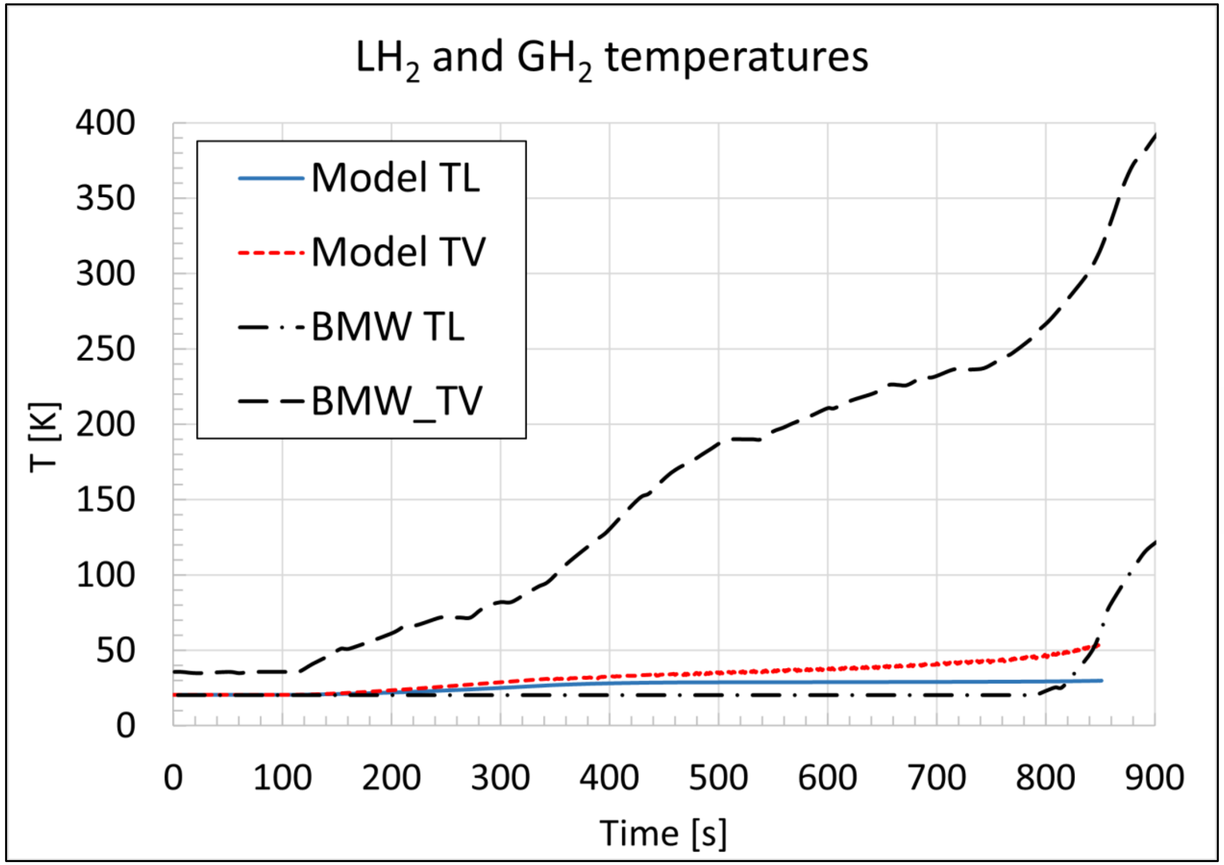


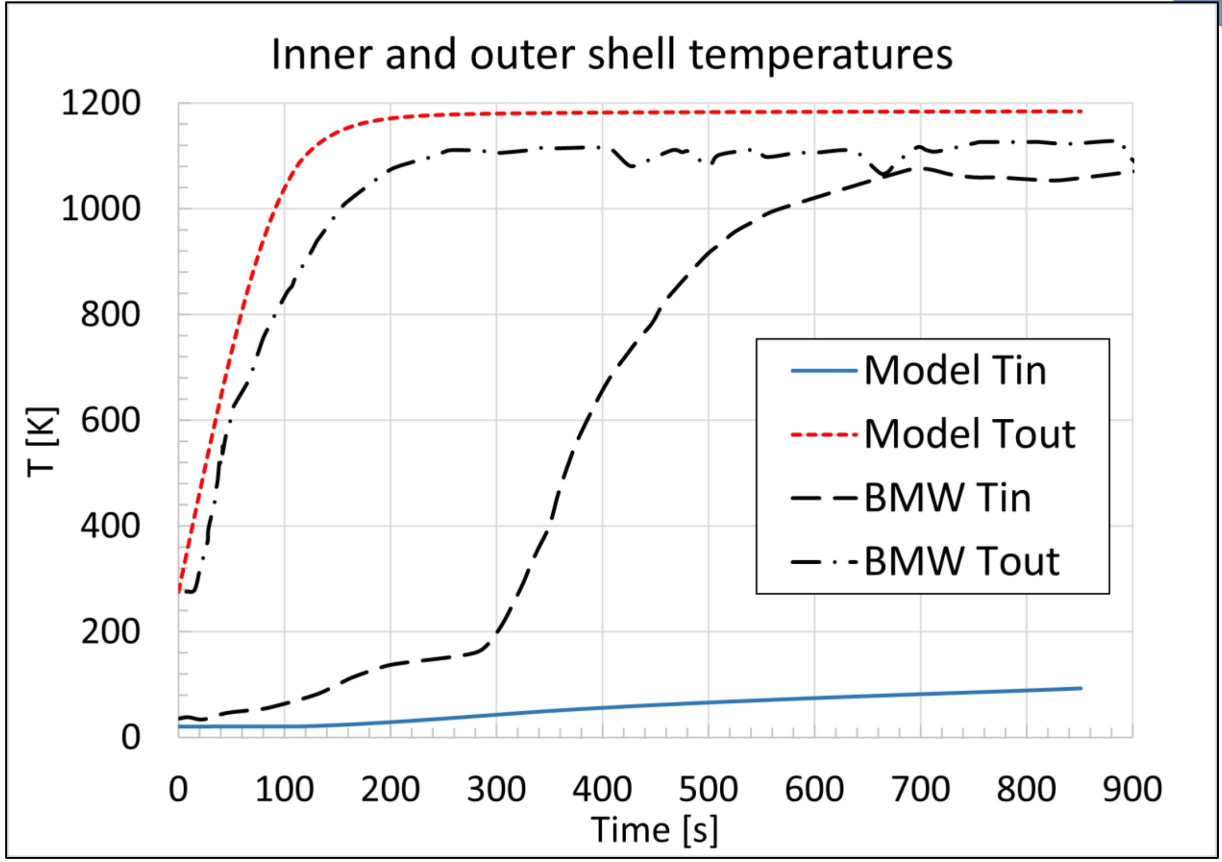


- Estimated tank pressure and LH_2 level approximate well the measurements
- Complete hydrogen venting after 854 s (model) instead of 900 s (exp.)

Fire test

Lumped model - Results





Estimated temperatures do not agree with experimental results due to the thermal nodes approach.

Fire test

[Ustolin, F., Iannaccone, T., Cozzani, V., Jafarzadeh, S., Paltrinieri, N., 2021. Time to Failure Estimation of Cryogenic Liquefied Tanks Exposed to a Fire, in: 31st European Safety and Reliability Conference. pp. 935–942]

Lumped model - SH2IFT

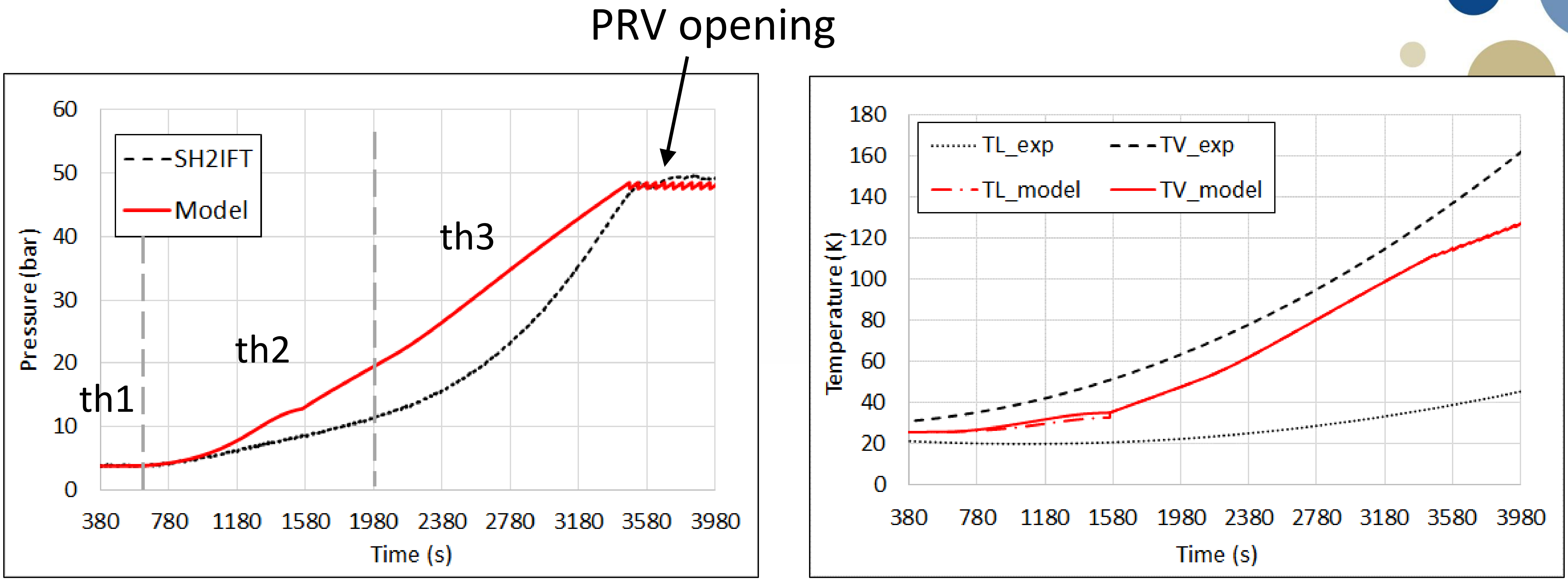
Initial conditions

Parameter	Units	Value
Tank filling degree	%	38
Tank pressure	bar	3.78
PRV pressure open	bar	48,5
PRV pressure close	bar	47.5
Ambient temperature	K	293
Flame temperature	K	1073
LH_2 temperature	K	25.8
H_2 temperature	K	25.8

- **Tank volume**: 1m^3
- **Tank internal diameter**: 925 mm
- **Tank insulation thickness**: 70 mm
- **Tank length**: 1,488 mm
- **Initial H2 mass**: 27 kg (24 kg LH2)
- **Estimated PRV diameter**: 10.8 mm
- **MLVI thermal conductivity (assumed)**:
  - **th1** = 1.5 mW/m K (t < 272 s)
  - **th2** = 109 mW/m K (272 < t < 1,727 s)
  - **th3** =160 mW/m K (t > 1,727 s)

Fire test

Lumped model - SH2IFT



MLVI thermal conductivity changed according to tank and vacuum press.

Simulation time: ~20 minutes

Fire test

CFD analysis - Methodology

- **Type**: 2D
- **Software**: Ansys Fluent
- **Multiphase model**: Volume of Fluid
- **Turbulence model**: k-omega SST
- **Evaporation-condensation model**: Lee (Hertz-Knudsen)
- **Pressure-velocity coupling algorithm**: SIMPLEC
- **Thermodynamic properties**: implemented from NIST database
- **Symmetry**: axial

Fire test

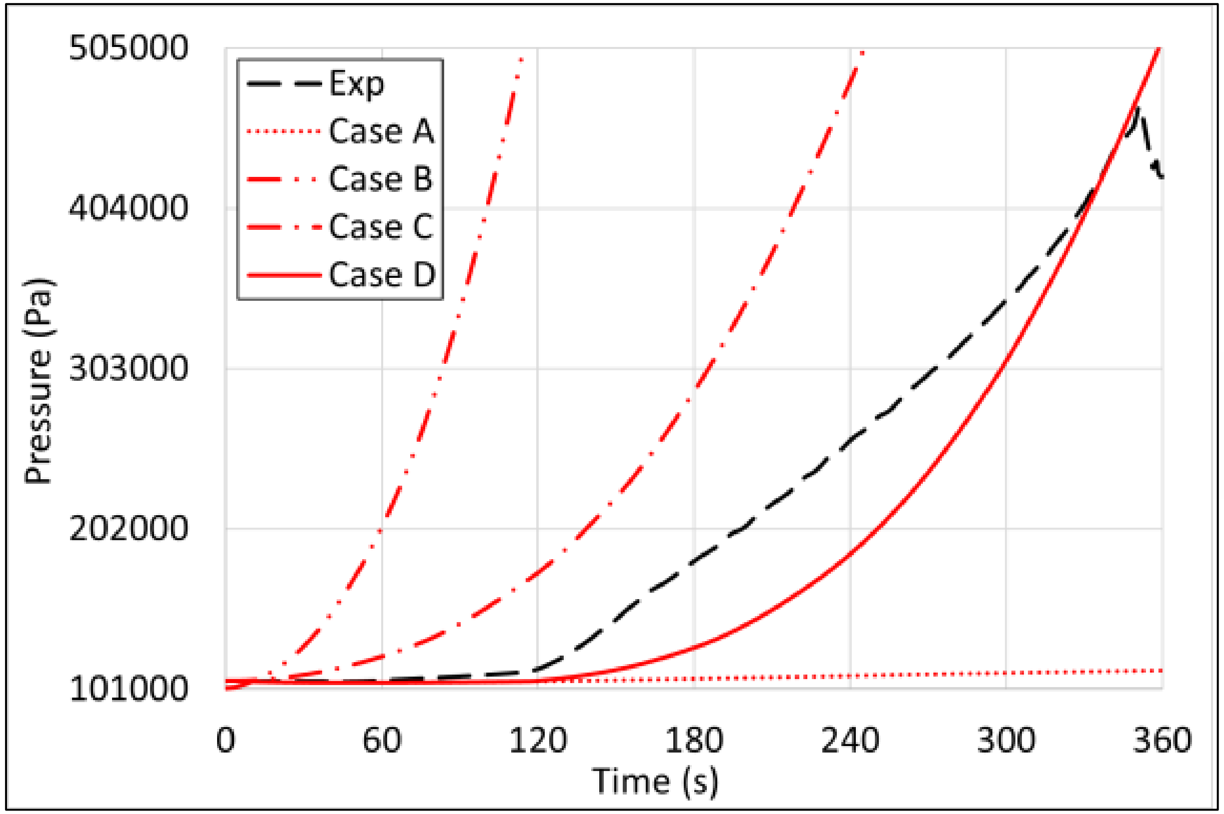
CFD analysis - Assumptions

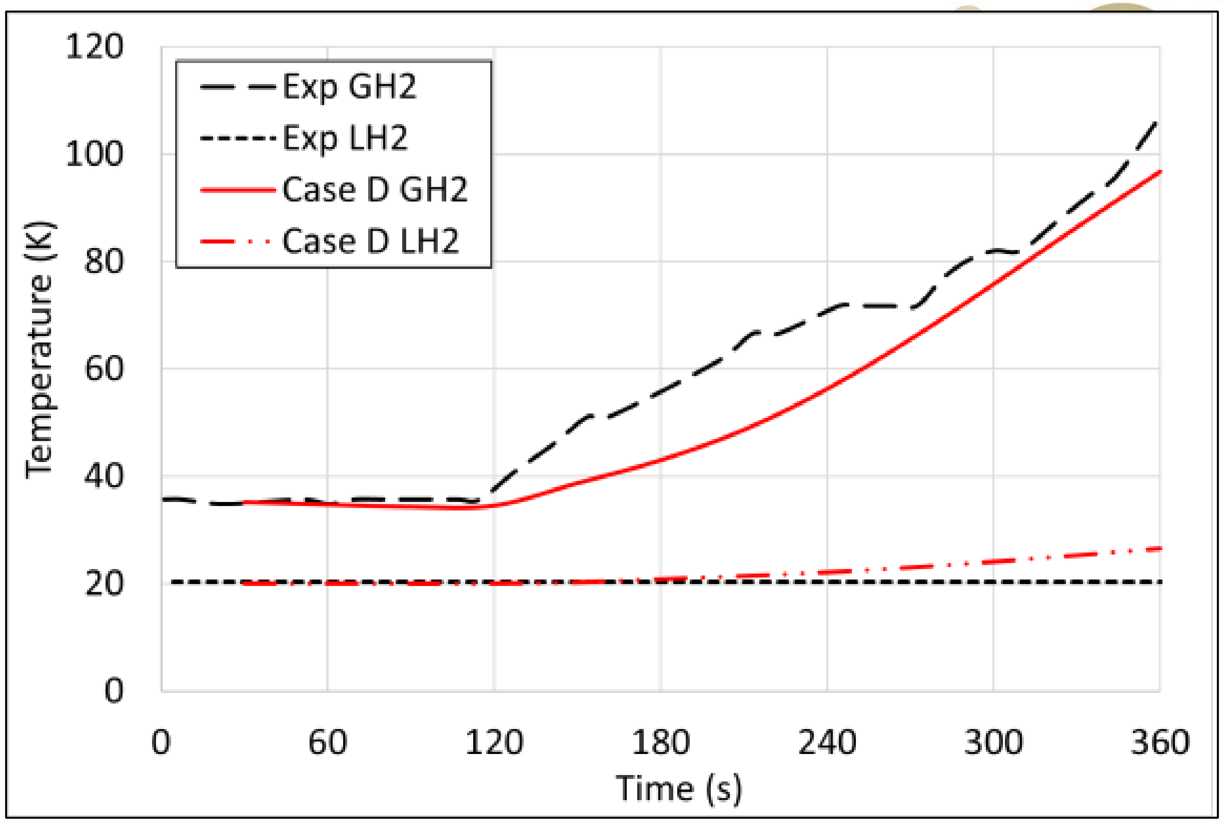
- **Tank diameter:** 460 mm
- **MLVI properties**
  - **Thermal conductivity**: 1.5, 160.0, 239.0 mW/m K
  - **Density**: 167 kg/m^3
  - **Layer density**: 23 layers/cm

MLVI thermal conductivity was changed from **1.5** to **160.0 mW/m K** at the simulated time of **115 s** in case D

Fire test

CFD analysis - Results



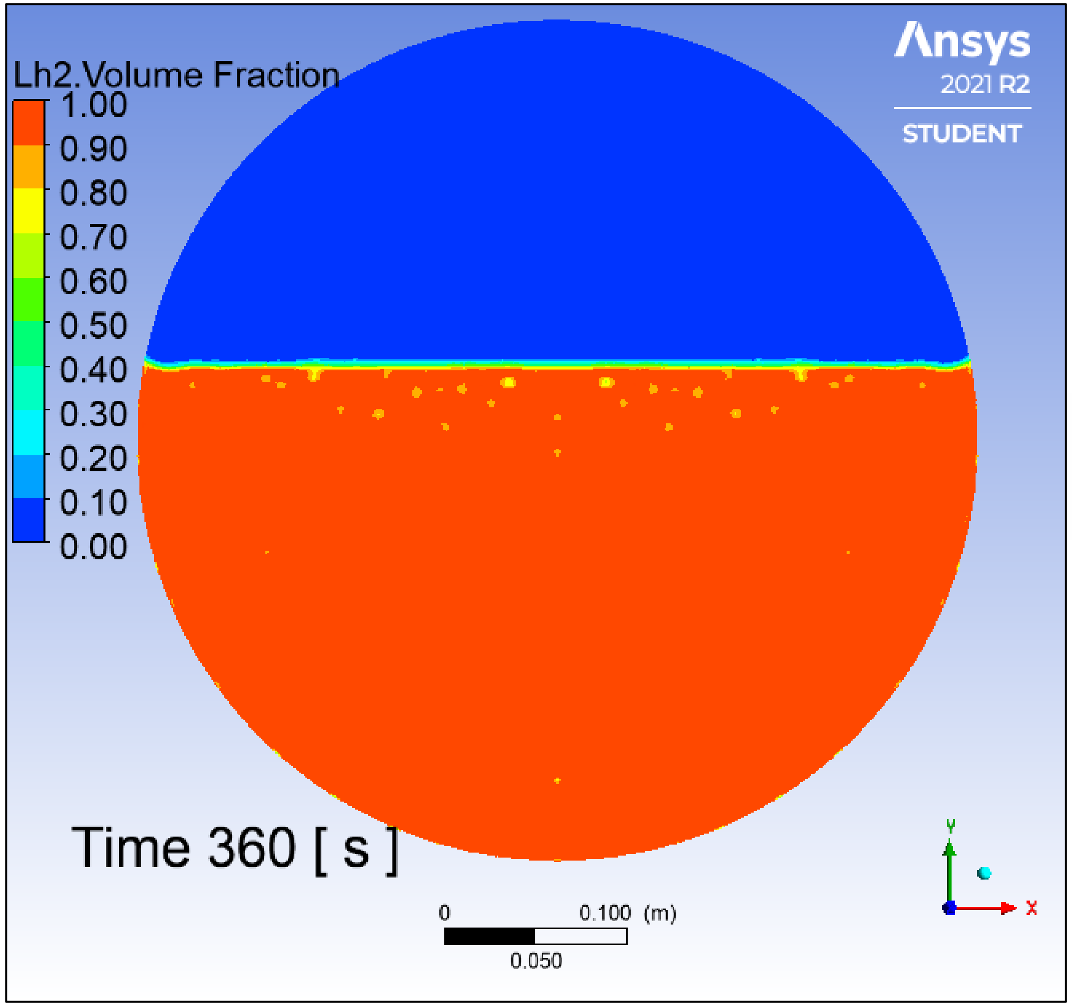


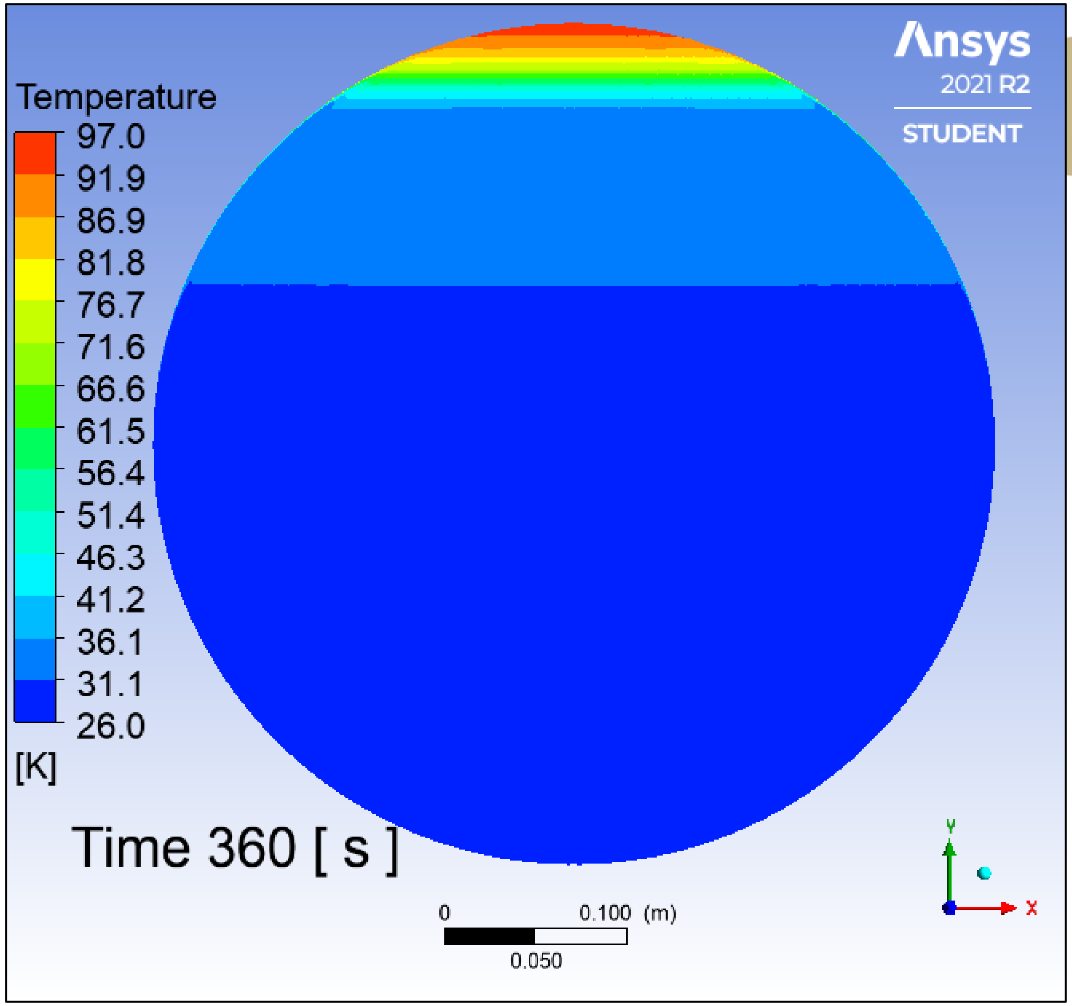
Case A: 1.5 mW/m K **Case B**: 239.0 mW/m K **Case C**: 160.0 mW/m K

Case D: 1.5 mW/m K if t<115 s; 160.0 mW/m K if t>115 s

Fire test

CFD analysis - Results

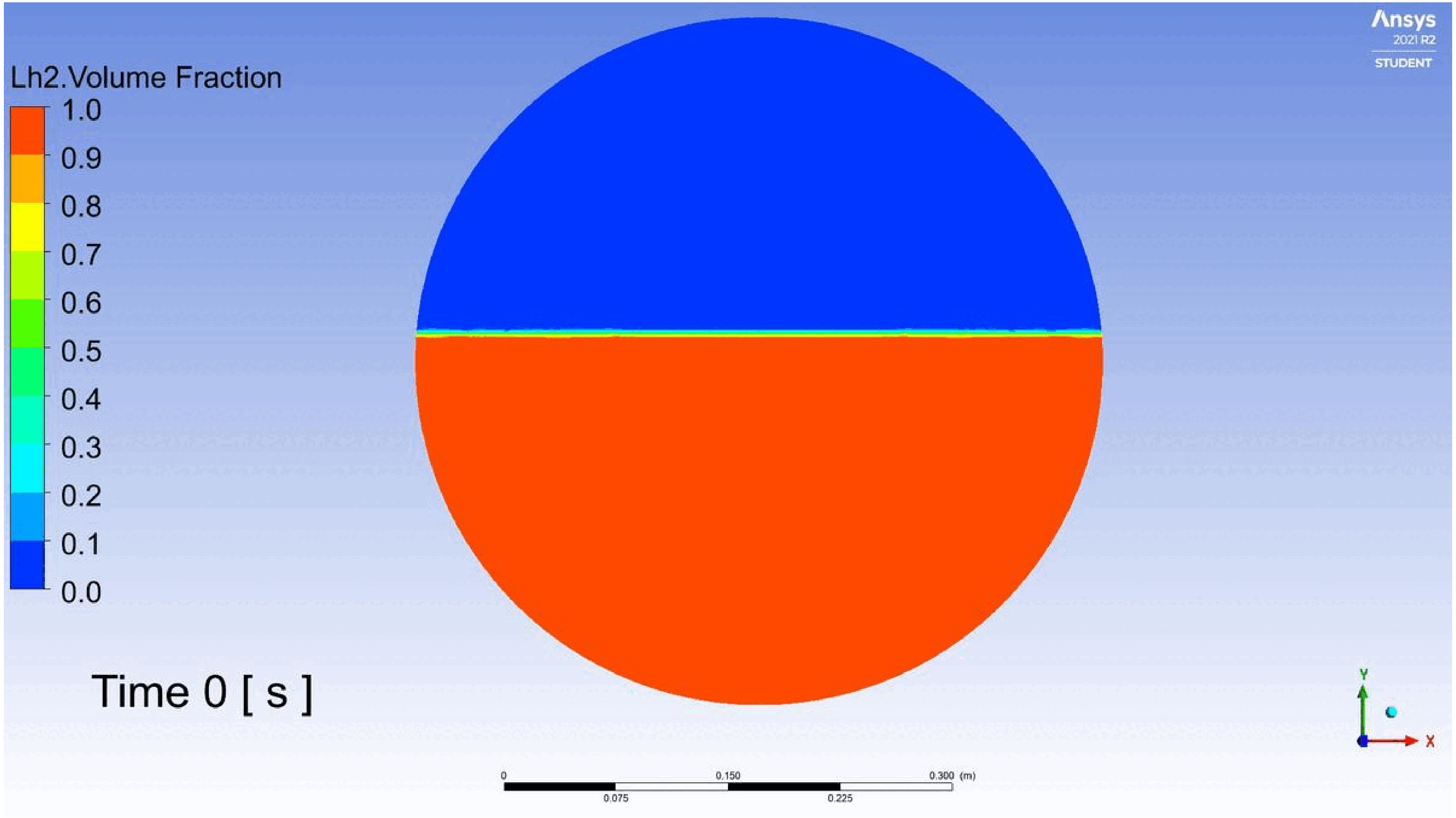




Case D: 1.5 mW/m K if t<115 s; 160.0 mW/m K if t>115 s

Fire test

CFD analysis - Results



Fire test

Consequences of an LH_2 BLEVE

Methods: BLEVE consequences (blast wave, fragments range, fireball) were simulated by means of:

1. Integral models

- Mechanical energy
- Overpressure and impulse
- Missiles range

2. Numerical model (CFD)

- Blast wave (no combustion)

Integral models - Methodology

Methods: theoretical models for mechanical energy

Proposed by	Equation
Brode (1959)	$E_{Brode} = \frac{P - P_0}{\gamma - 1} V^*$
Smith and Van Ness (1996)	$E_{IE} = P \cdot V^* \cdot \ln \frac{P}{P_0}$
Crowl (1992, 1991)	$E_{TA} = P \cdot V^* \left[\ln\left(\frac{P}{P_0}\right) - \left(1 - \frac{P_0}{P}\right) \right]$
Prugh (1991)	$E_{Prugh} = \frac{P \cdot V^*}{\gamma - 1} \left(1 - \frac{P_0}{P}\right)^{\frac{\gamma - 1}{\gamma}}$
van den Bosch and Weterings (2005)	$E_{TNO} = m_V (u_V - u_{V_{is}}) + m_L (u_L - u_{L_{is}})$
Planas-Cuchi et al. (2004)	$E_{Planas} = -[(u_{L0} - u_{V0}) m_T \cdot x - m_T \cdot u_{L0} + U_i]$
Casal and Salla (2006)	$E_{SE} = k \cdot m_L (h_L - h_{L0})$
Genova et al. (2008)	$E_{Genova} = \psi \cdot m_L \cdot c_{p,L} (T_L - T_{L0})$
Birk et al. (2007)	$E_{Birk} = m_V (u_V - u_{V_{is}})$

Ideal gas behaviour models (Brode, Smith and Van Ness, Crowl, Prugh)

Real gas behaviour models (van den Bosch and Weterings, Planas-Cuchi et al., Casal and Salla, Genova et al., Birk et al.)

Blast wave overpressure and impulse (far field):

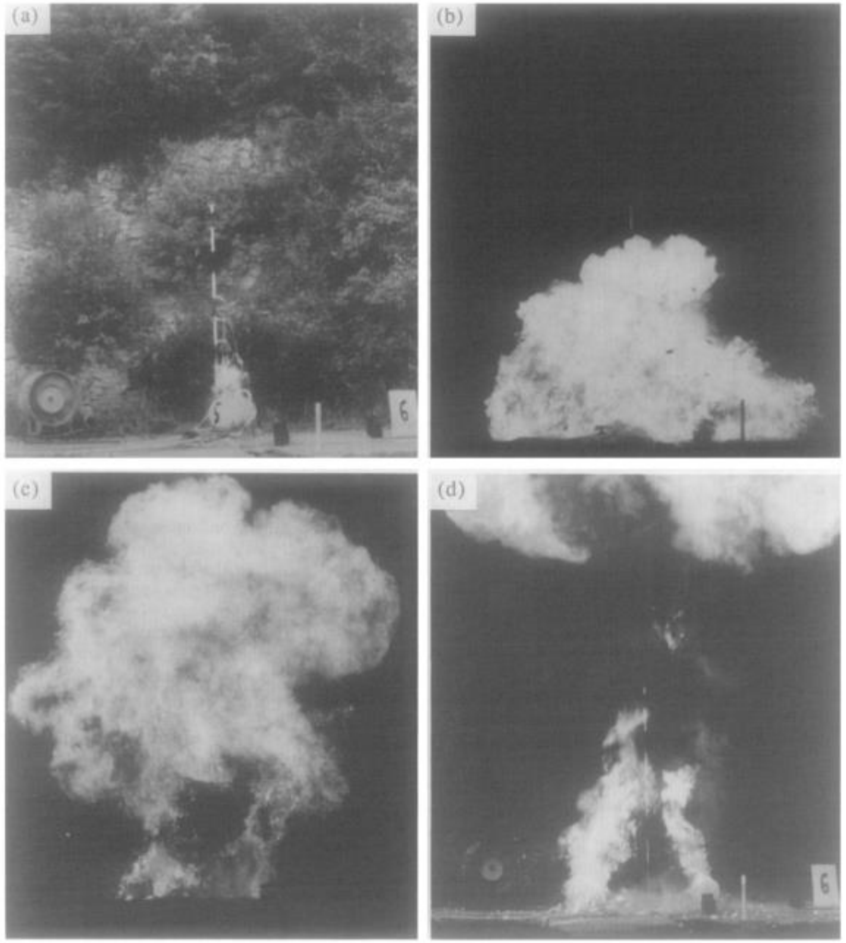
- ➢ TNT equivalent mass
- ➢ Sachs scaling law (Baker curves)

Safety distance → $P < 1.35$ kPa

Integral models - Assumptions

Ten LH2 vessels with different H2 content and initial pressure and temperatures were tested by BMW

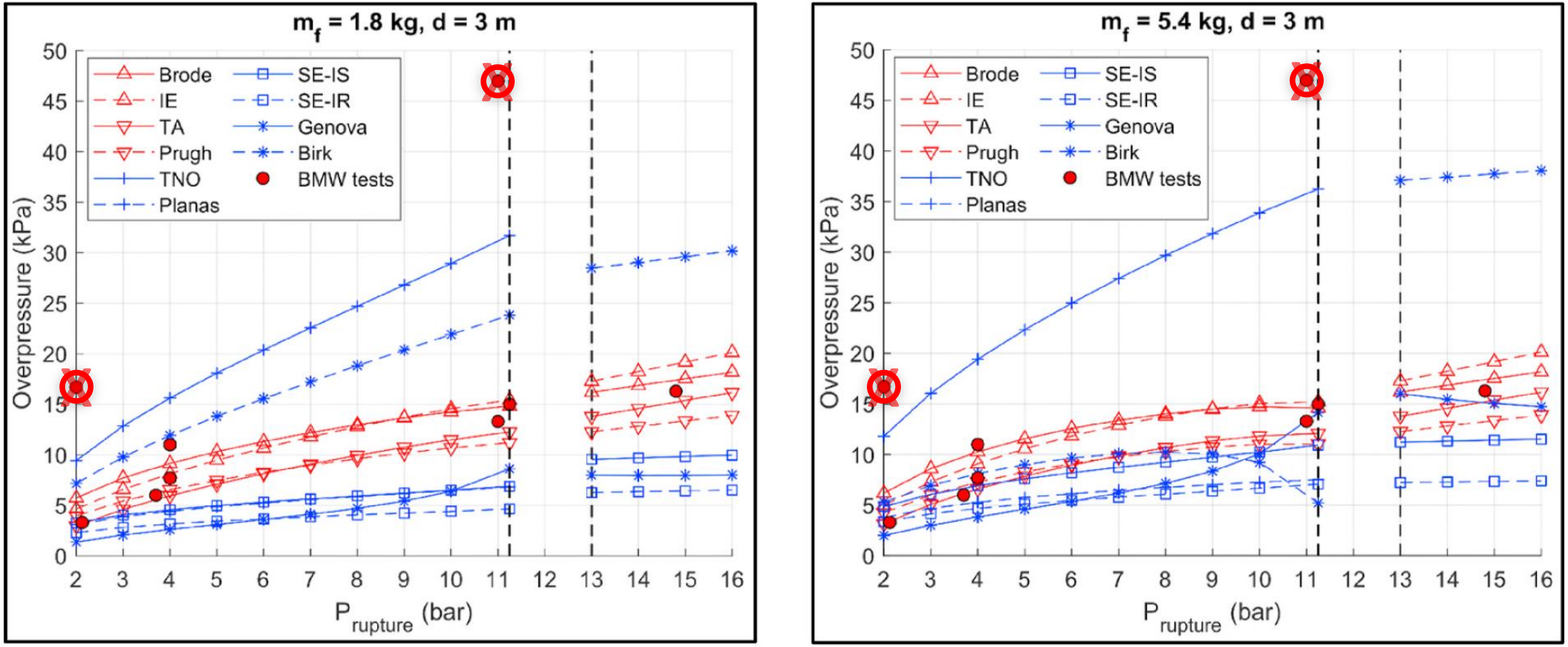
- **Tank volume:** 0.120 m^3
- **Rupture pressure**: 2, 4, 11 and 15 bar
- **Temperature (LH2, GH2)**: saturation
- **Hydrogen mass**: 1.8, 5.4 kg



BLEVE

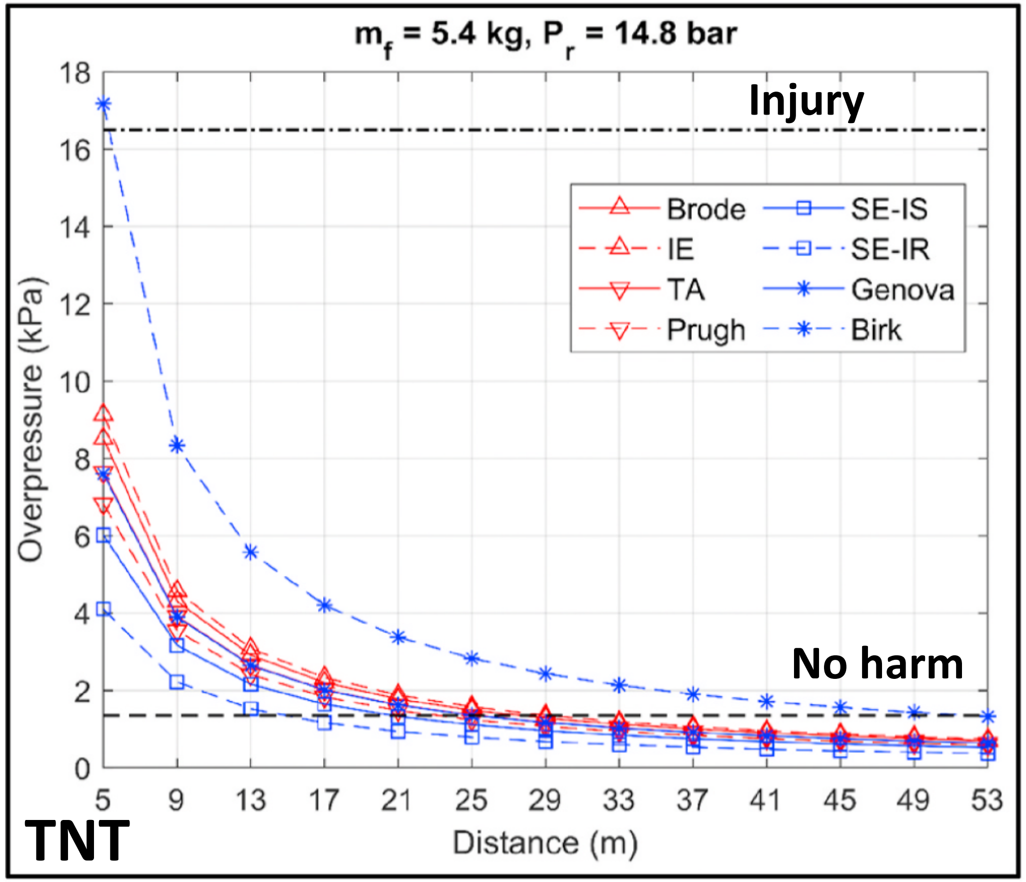
[Pehr, K., 1996. Aspects of safety and acceptance of LH2 tank systems in passenger cars. Int. J. Hydrogen Energy 21, 387–395]

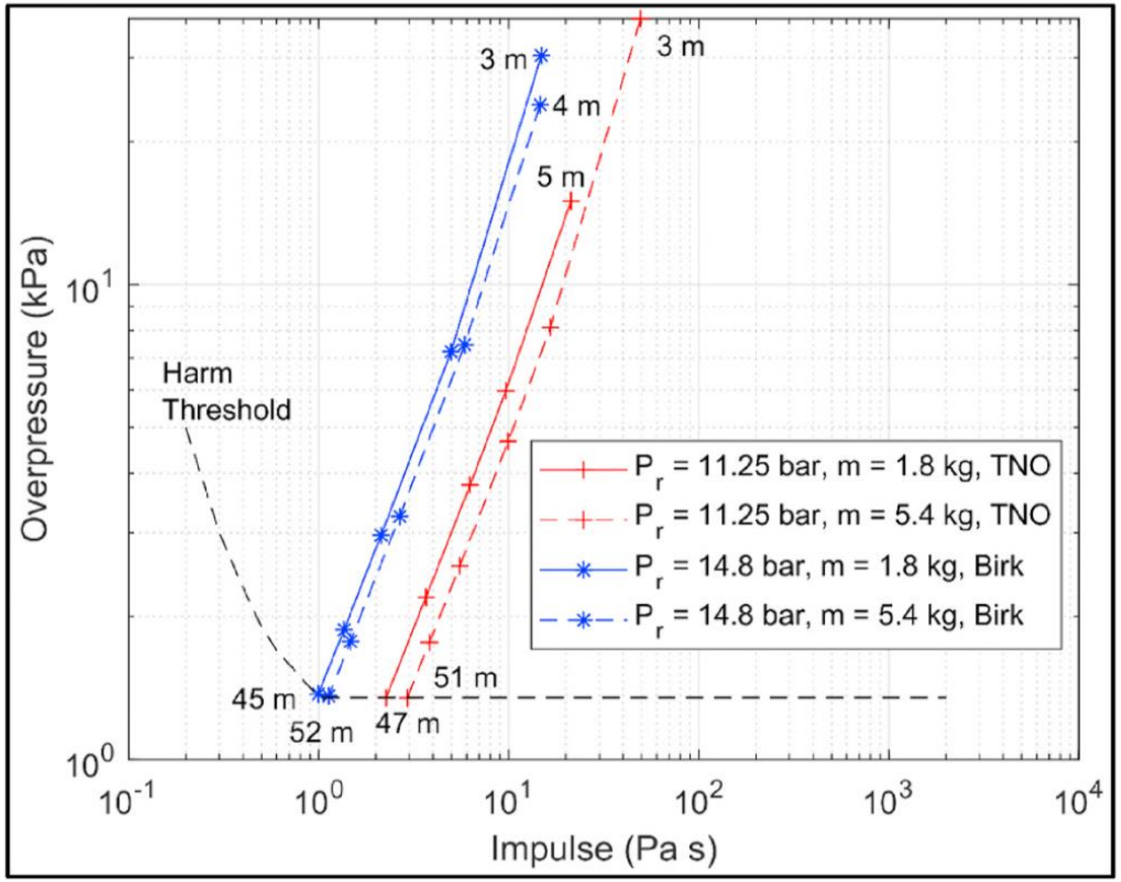
Integral models - Results



TNT equivalent mass to convert mechanical energy to overpressure

Integral models - Results





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ELSEVIER

An innovative and comprehensive approach for the consequence analysis of liquid hydrogen vessel explosions

BLEVE

Integral models (combustion)

1. Ideal and real gas behaviour models (mechanical energy)

2. Combustion process (chemical energy): methodology proposed by Molkov and Kashkarov (2015) for pressurized H2 tanks:

$$E_{ch} = \beta \cdot \left(\frac{r_{sh}}{r_b}\right)^3 \cdot LHV$$

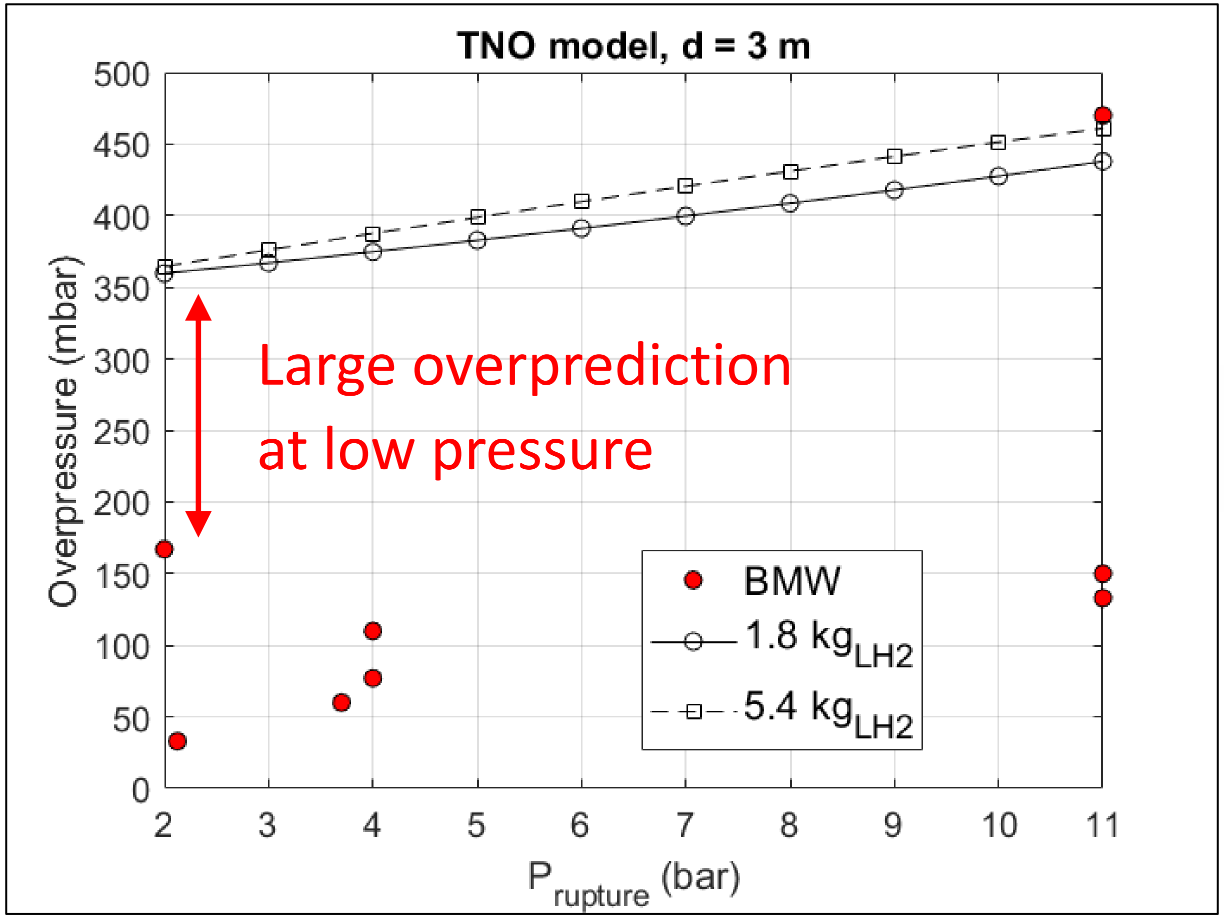
$$\beta = 0.052$$

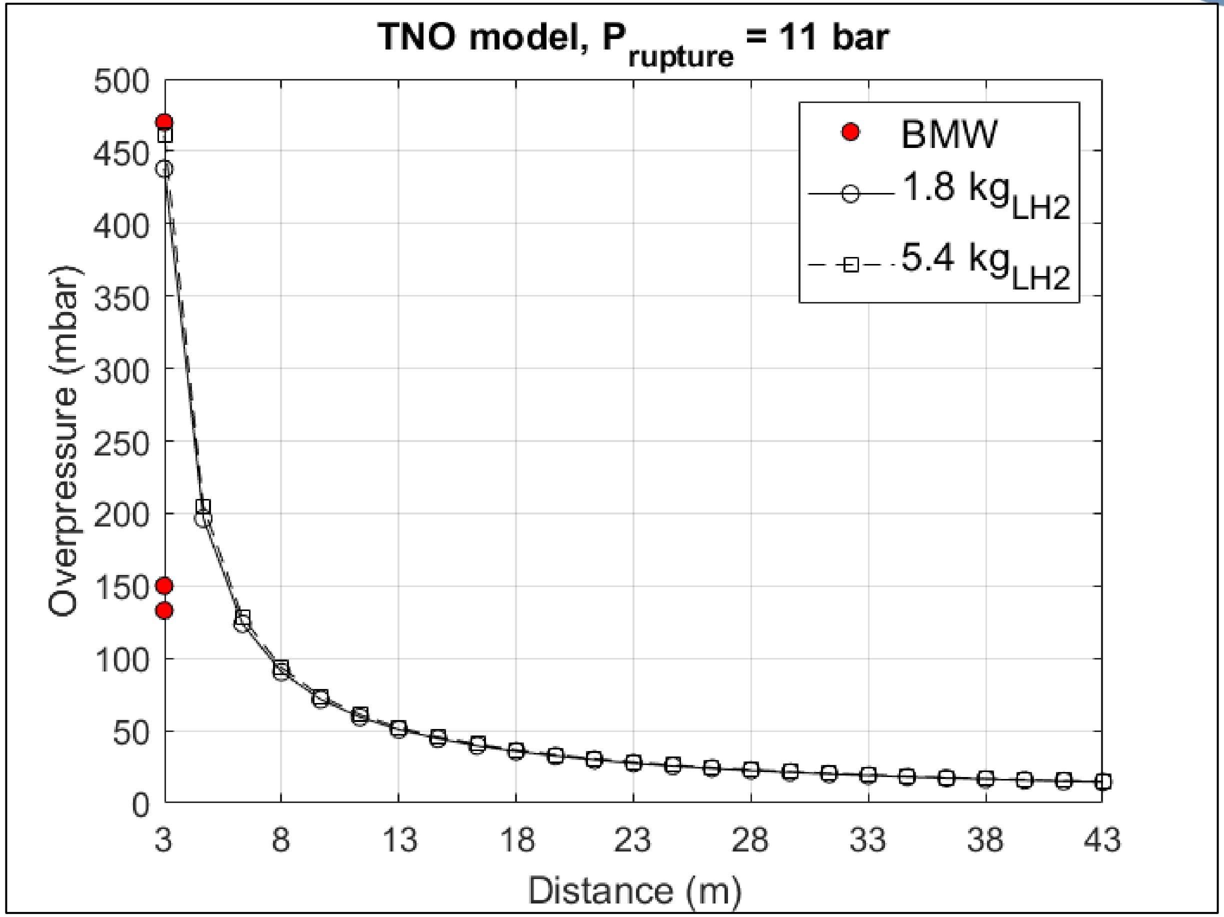
$$E_{TOT} = \alpha \cdot E_{mech} + E_{ch}$$

3. Therefore, the total energy (mechanical + chemical) is estimated

BLEVE

Integral models (combustion) - Results





Most conservative model: TNO

Overestimation at low pressure (2, 4 bar)

BLEVE

CFD analysis

Methods: CFD analysis of the BLEVE explosion by means of the ADREA-HF in-house 3D time dependent finite volume code (activity of the visiting period at NCSR "Demokritos").

- **Multiphase flow model**: Homogeneous Equilibrium Model (HEM)
- **Raoult's law** is used for the components phase distribution
- **Turbulence model**: standard k-ε model with wall functions

Aim: reproduce the BMW bursting scenario tests by means of a parametric analysis (LH_2 mass, tank pressure and temperature).

CFD analysis

Configurations

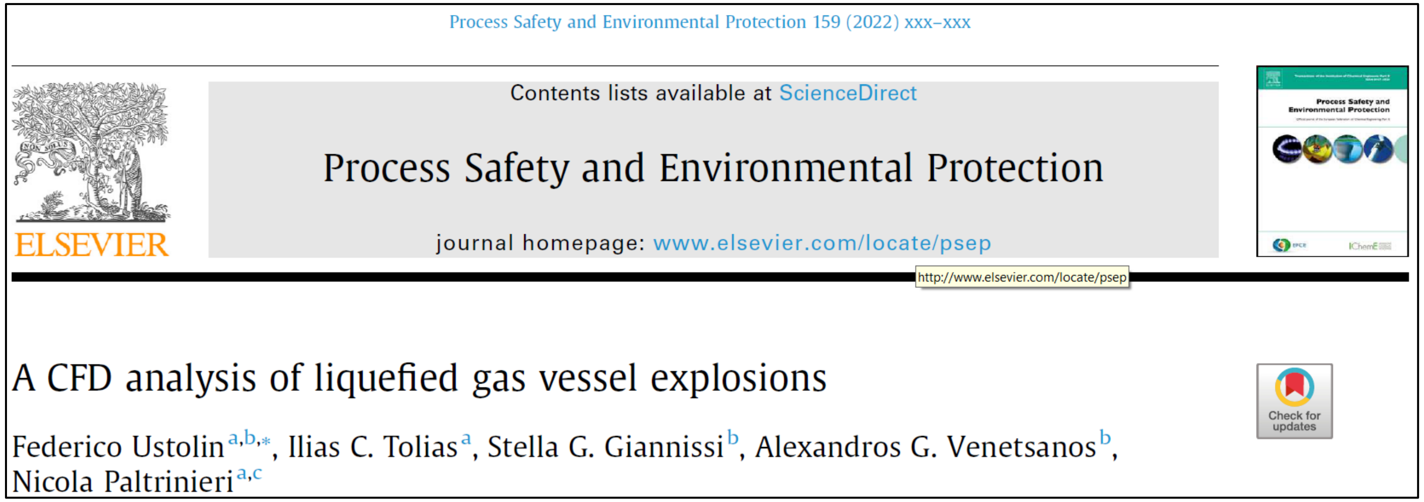
- Pressure levels: 4, 11 and 15 bar
- The tank was simulated either full of liquid or gaseous H_2
- **Filling degree**: 37% only at 11 bar
- The model was first validated with CO_2 BLEVE experiments [56]
- The focus was placed on the dynamic of the BLEVE blast wave (no combustion).

BLEVE

CFD analysis

Main finding on dynamic of pressure wave.
Influence on the overpressure and impulse of:

- hydrogen liquid and gaseous phase
- hydrogen mass
- initial temperature and pressure



Process Safety and Environmental Protection 159 (2022) xxx–xxx

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A CFD analysis of liquefied gas vessel explosions

Federico Ustolin[a,b,*], Ilias C. Tolias[a], Stella G. Giannissi[b], Alexandros G. Venetsanos[b], Nicola Paltrinieri[a,c]

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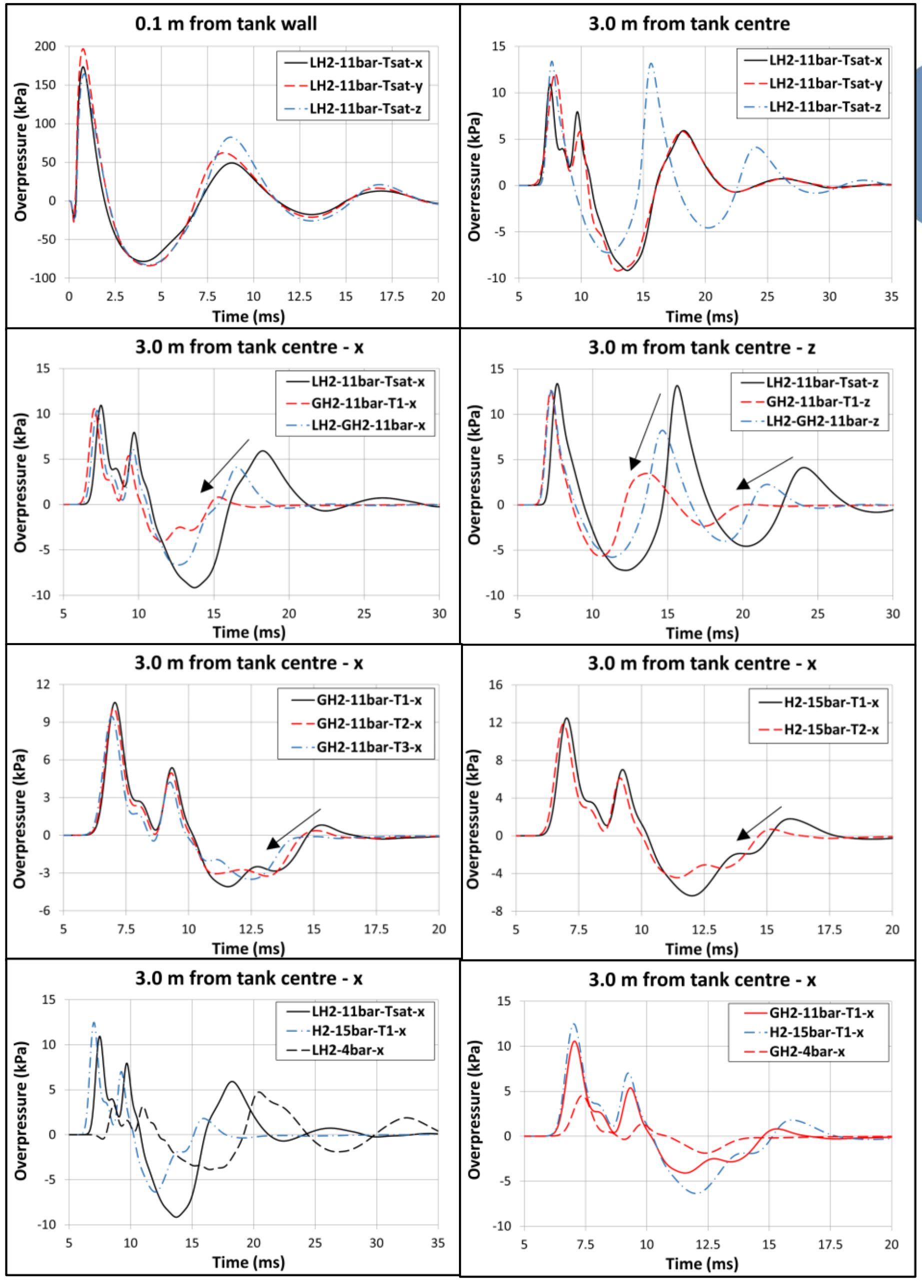
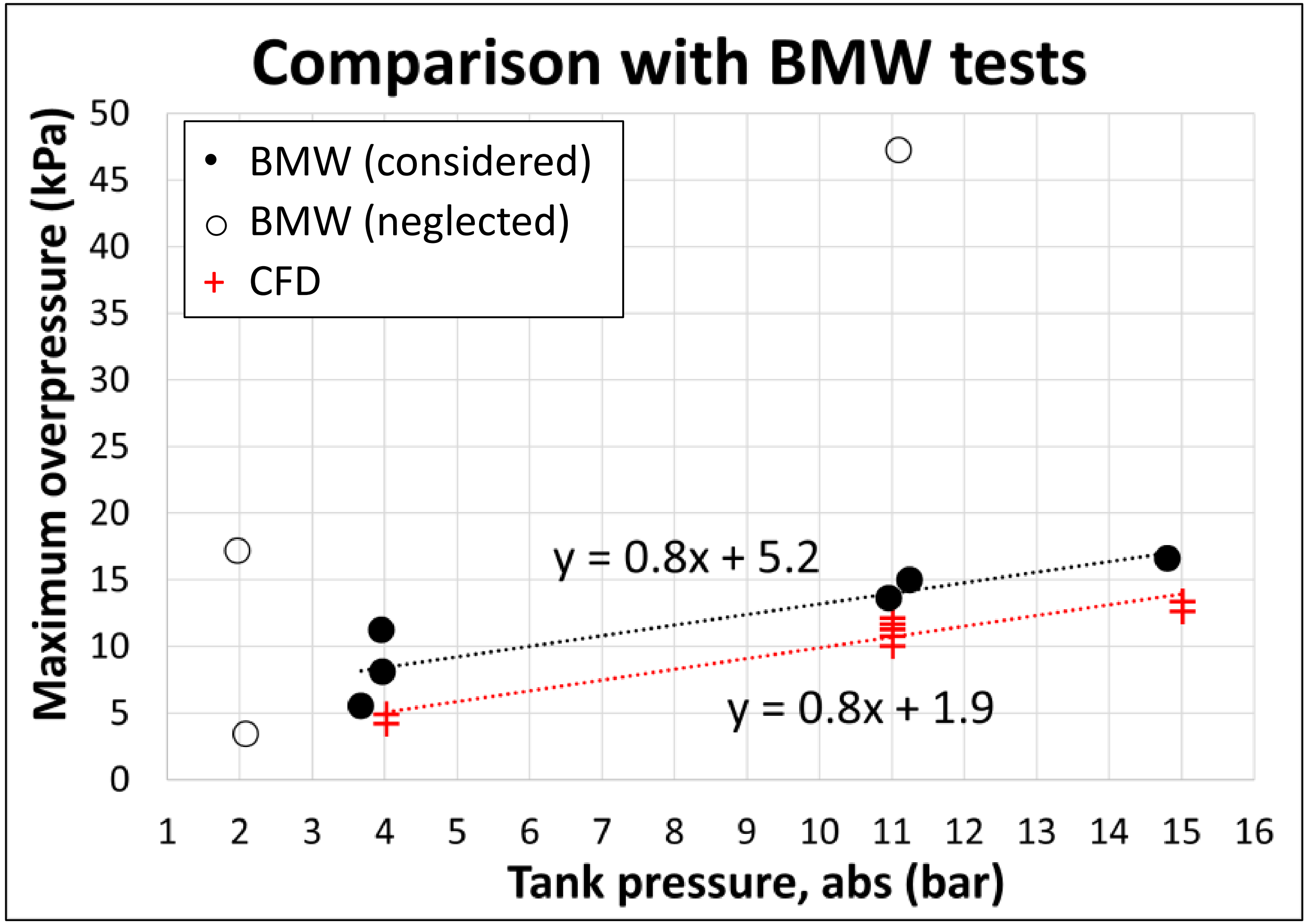


BLEVE

LH_2 BLEVE CFD analysis



Speculation: the difference in overpressure is caused by the combustion (not simulated)

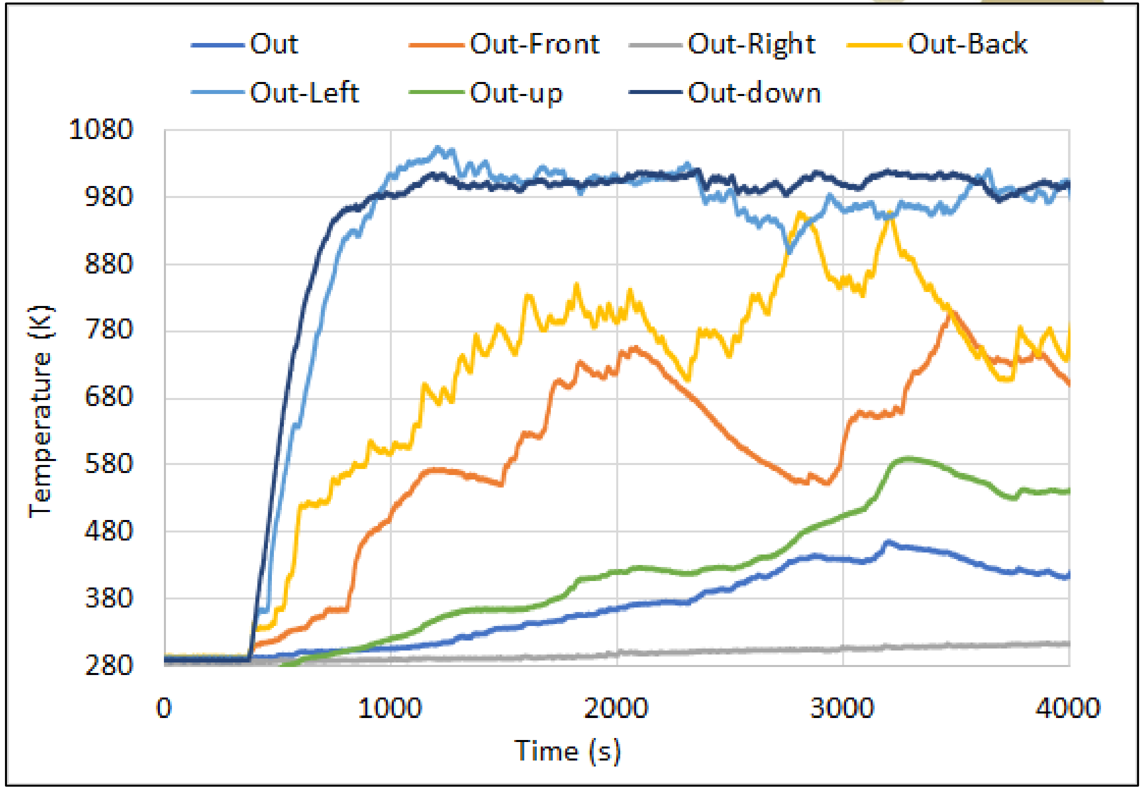
BLEVE

SH2IFT project LH2 BLEVE test

BLEVE

Discussion & conclusions

- ✓ Conditions in outdoor medium-scale experiments are difficult to control
- ✓ Developed models show good agreement with experiments
- ✓ Lumped and integral models are good starting points for developing more accurate models



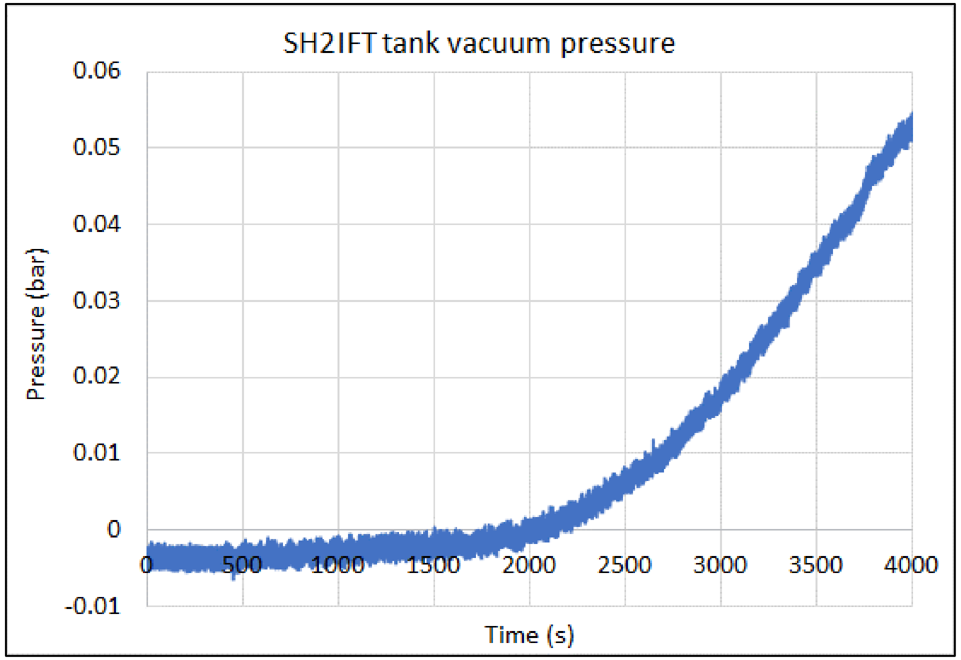
Temperatures measured in different positions on the outer LH2 tank shell during the SH2IFT fire test

Discussion & conclusions

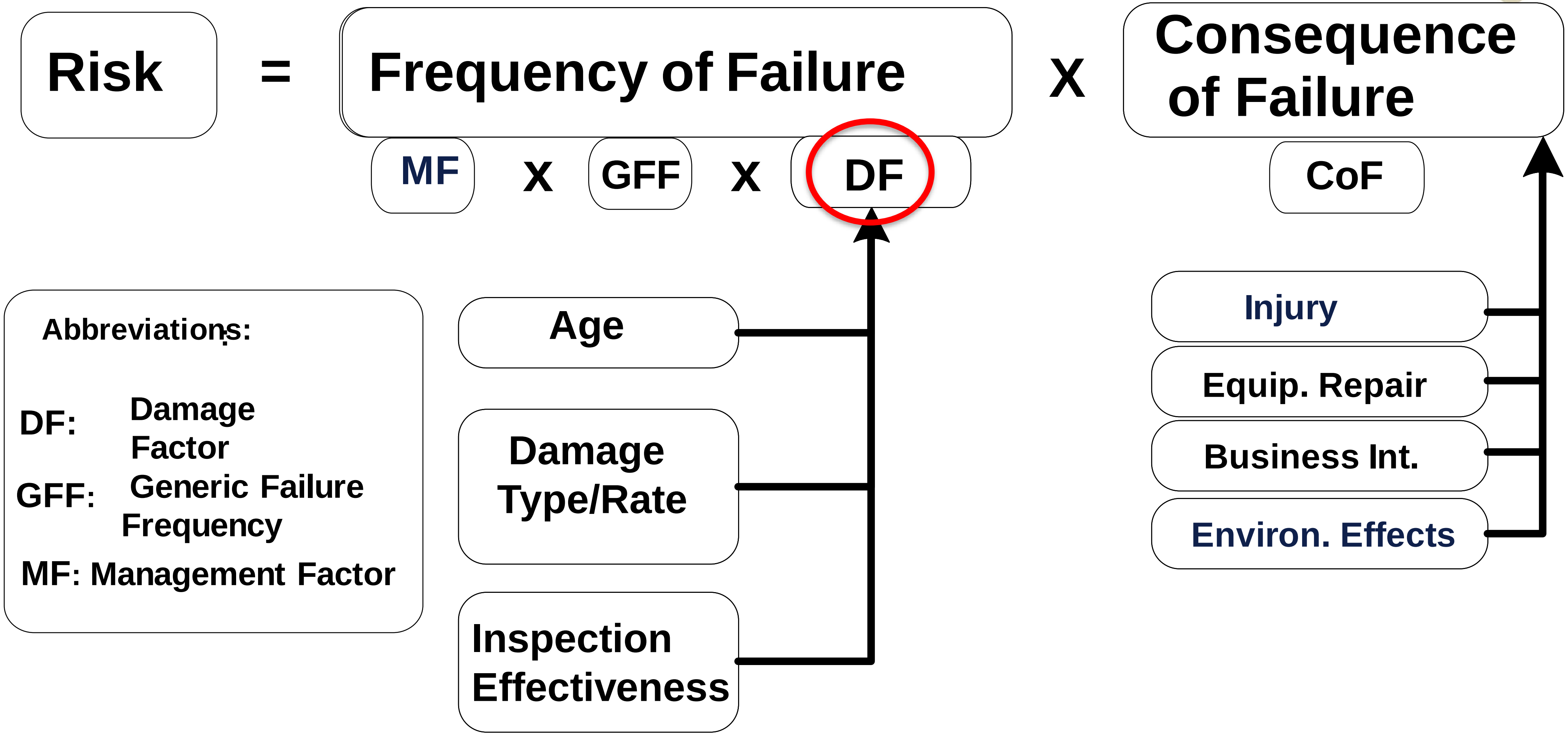
- ✓ Material behaviour (e.g. tank insulation) exposed to fire must be investigated
- ✓ Initial conditions (e.g. LH2 and GH2 mass) must be known
- ✓ Combustion process must be considered for LH2 BLEVE blast wave assessment

Proposed safety barrier:

- Supply of subcooled LH2
- Nets for fragments

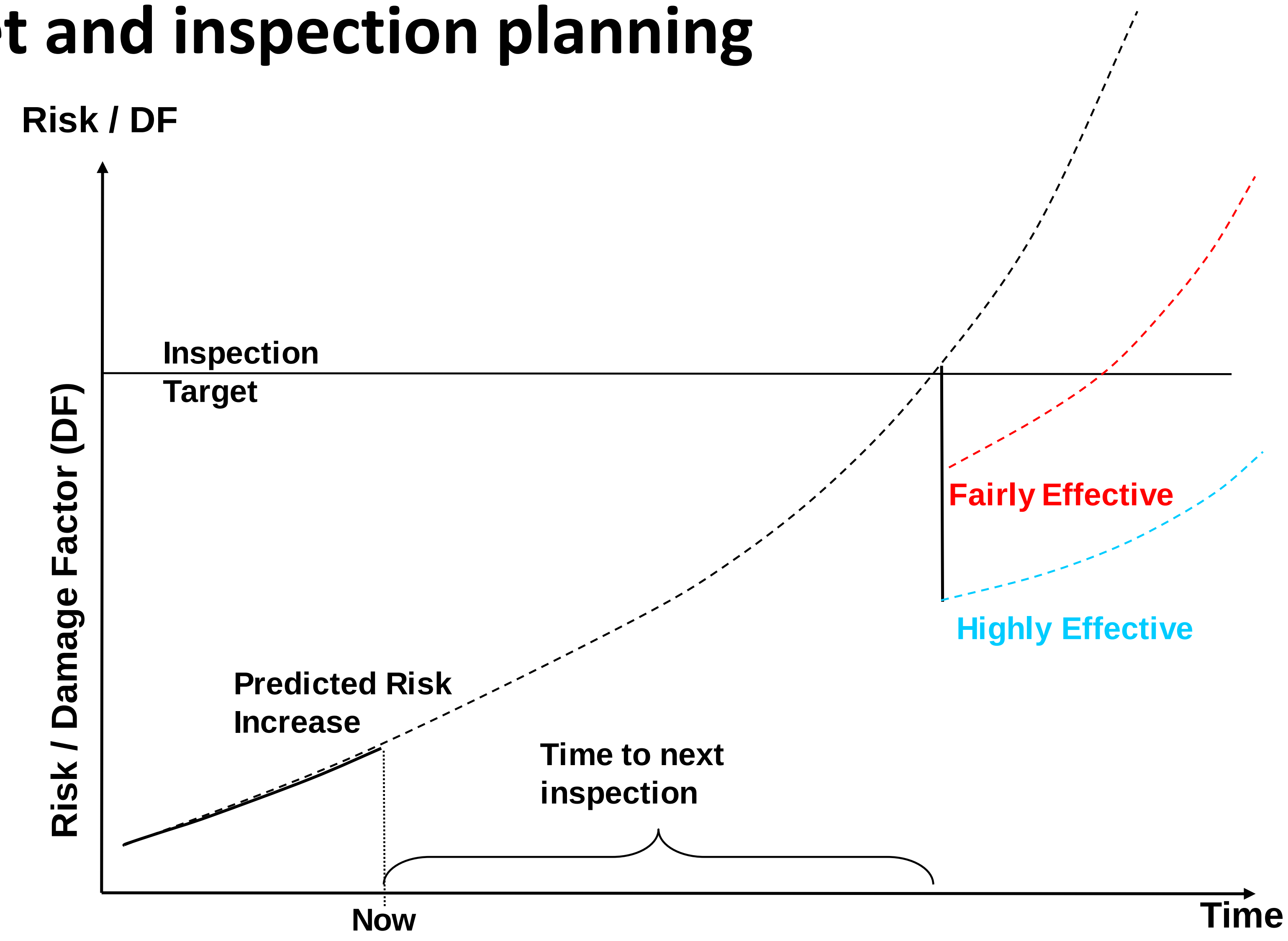


Risk definition



Support for inspection and maintenance

Risk target and inspection planning



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Support for inspection and maintenance

Consolidated standards on inspection planning (and subsequently maintenance) based on quantitative risk assessment (risk-based inspection -RBI- methodology):

- API 580/581,
- DNV RP G101
- EN16991:2018

Few hydrogen-related degradation mechanisms to define the damage factors are considered

The introduction of hydrogen-specific mechanisms into quantitative risk methods used for planning inspection and maintenance activities would boost accident prevention.

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[Ustolin, F., Paltrinieri, N., Berto, F., 2020. Loss of integrity of hydrogen technologies: A critical review. Int. J. Hydrogen Energy 45, 23809–23840. https://doi.org/https://doi.org/10.1016/j.ijhydene.2020.06.021]

RBI planning for hydrogen technologies

1. Review of current RBI standards and recommended practises

Table 1. Risk-based inspection standards in literature.

Standard	Ref.	Title	Year
API 580	[12]	Risk Based Inspection	2016
API 581	[13]	Risk Based Inspection methodology	2016
ASME PCC-3	[15]	Inspection Planning Using Risk-Based Methods	2017
DNVGL-RP-G101	[8]	Risk based inspection of offshore topsides static mechanical equipment	2017
EN16991	[14]	Risk-based inspection framework	2018

2. Metal-hydrogen interactions, loss of integrity (LOI) phenomena and their mechanisms

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Loss of integrity (LOI) phenomena and mechanisms

Table 2. Comparison between examples of damages provided by the EN16991 standard [14], and the loss of integrity (LOI) phenomena for hydrogen technologies [5].

LOI phenomena	EN16991
Hydrogen damages (HD):	
○ Hydrogen embrittlement (H_2 environment embrittlement, H2 stress cracking, loss in tensile ductility)	Embrittlement incl. hardening, strain aging, temper embrittlement, liquid metal embrittlement, etc. (general)
○ Hydrogen attack (HA)	High temp. HA (H_2 induced damage)
○ Blistering	Blistering (H_2 induced damage)
○ Shatter cracks, flakes, fisheyes	Cracking, mainly on surface (general)
○ Microperforation	Micro-cracking (general)
○ Degradation in flow properties	Fluid flow disturbance (general)
○ Metal hydride formation	Dealloying (general)
Low temp. embrittlement	Embrittlement (general)
Thermal contraction, stresses caused by: ○ dimensional change ○ thermal gradients	Dimensional changes, thermal fatigue (general)

A discussion about the mechanical and thermal fatigue was also provided.

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Projects on hydrogen safety

1. **SH$_2$IFT**: Safe Hydrogen Fuel Handling and Use for Efficient Implementation
2. ***PRESLHY** : PRENORMATIVE RESEARCH FOR SAFE USE OF LIQUID HYDROGEN

   * Collaboration during visiting
3. **H2 CoopStorage**: Development of tools enabling the deployment and management of a multi-energy Renewable Energy Community with hybrid storage
4. **SH$_2$IFT 2** : follow-up of SH$_2$IFT

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5. **SUSHy**: SUStainability development and cost-reduction of hybrid renewable energies powered Hydrogen stations by risk-based multidisciplinary approaches

Thank you for your attention






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QUESTIONS?