University of ULSTER

HySAFER

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H2FC Cyber-Laboratory: Open access engineering and modelling tools

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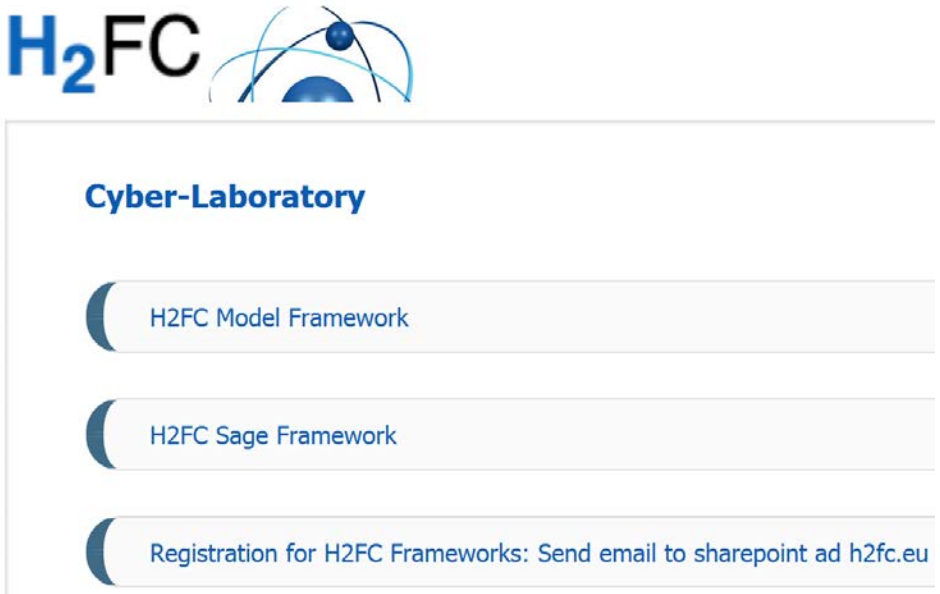
H2FC Cyber-Laboratory

- Goal: ***Defragmentation*** and improvement of the e-infrastructure for hydrogen and fuel cell research.
- Development of a ***comprehensive***, properly ***validated*** and ***openly available*** set of software tools and models.
- Sustainability: Cyber-laboratory will be ***maintained*** and continuously ***updated*** (after the end of the H2FC project as a part of European ***e-Infrastructure*** for H2FC research)



Available engineering tools

- **Fuel Cells (CEA):**
  - Mass balance for a PEM Fuel Cell
- **Safety (UU):**
  - Hydrogen expanded jet parameters (ideal gas)
  - Hydrogen under-expanded jet parameters (real gas)
  - Free jet model for ideal gas (HSL)
  - Adiabatic blowdown of a storage tank
  - Isothermal blowdown of a storage tank
  - Pressure peaking phenomenon, constant flow rate (unignited)
  - Pressure peaking phenomenon, tank blowdown (unignited)
  - Flame length and three separation distances for jet fires
- **Storage (NCSRD):**
  - Gas Storage in Hydrates

Safety tools in development (UU)

- Calculation of maximum hydrogen concentration in an enclosure with one vent and steady-state release
- Vent sizing for deflagration in an enclosure fully filled by flammable hydrogen-air mixture
- Vent sizing for localised mixture deflagration in an enclosure
- Pressure peaking phenomenon for jet fires
- Blast wave decay from high-pressure tank rupture in a fire
- Calculation of fire resistance rating of storage tanks

Storage tools to be added (NCSRD)

- Design and Assessment of Storage Systems:
  - Acceptability envelope
  - System design (e.g. Hydride beds)
    - *http://hsecoe.srs.gov/models.html*

- Performance analysis and cost modelling:
  - Integrated Power Plant and Storage System Modelling
  - Material Operating Requirements
    - *http://hsecoe.srs.gov/technologyareas.html#performanceanalysis*
- Hydrogen Storage Systems Modelling and Analysis:
  - Compressed / Cryo-compressed tanks (liquid and gaseous)
  - Storage in metal-organic framework (MOF) materials
  - Systems that require off-board regeneration of the depleted material
    - *http://www.transportation.anl.gov/fuel_cells/hydrogen_storage_modelinganalysis.html*

Cyber-laboratory: an example of use

- Let us estimate what hazards are from currently available FC vehicles:
  - Deterministic separation distances at the open (three for jet fire from TPRD)
  - Fire resistance rating estimation (by blowdown time)
  - Pressure peaking phenomenon in a typical garage

Representative scenario:
Collision leading to opening of TPRD in FCH car (open air)

Parameter	Value (units)
Storage pressure	35 MPa [1]
Storage volume	0.171 m^3 [1]
TPRD diameter	1, 2, 3, 4.2 [2], 5 mm
Storage temperature	20^{O}C

1. Honda FCX specifications, http://www.hondaclarity.org/
2. Yohsuke, T. et al., "The spread of fire from adjoining vehicles to a hydrogen fuel cell vehicle", IJHE, 39, pp 6169-6175, 2014
3. Adams, P., "Identification of the optimum on-board storage pressure for gaseous hydrogen city buses", EIHP2, 2004
4. Yokoo, T., "Toyota's Development of Fuel Cell Hybrid Bus ("FCHV-BUS") and FCHV-BUS Business in Japan", 6th International Fuel Cell Bus Workshop, 4th June, 2009

Deterministic separation distances

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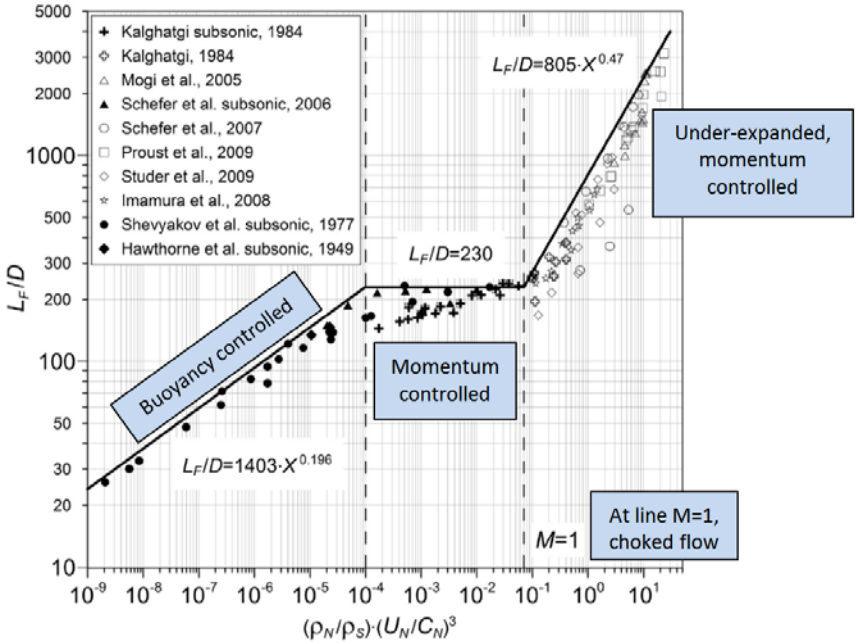
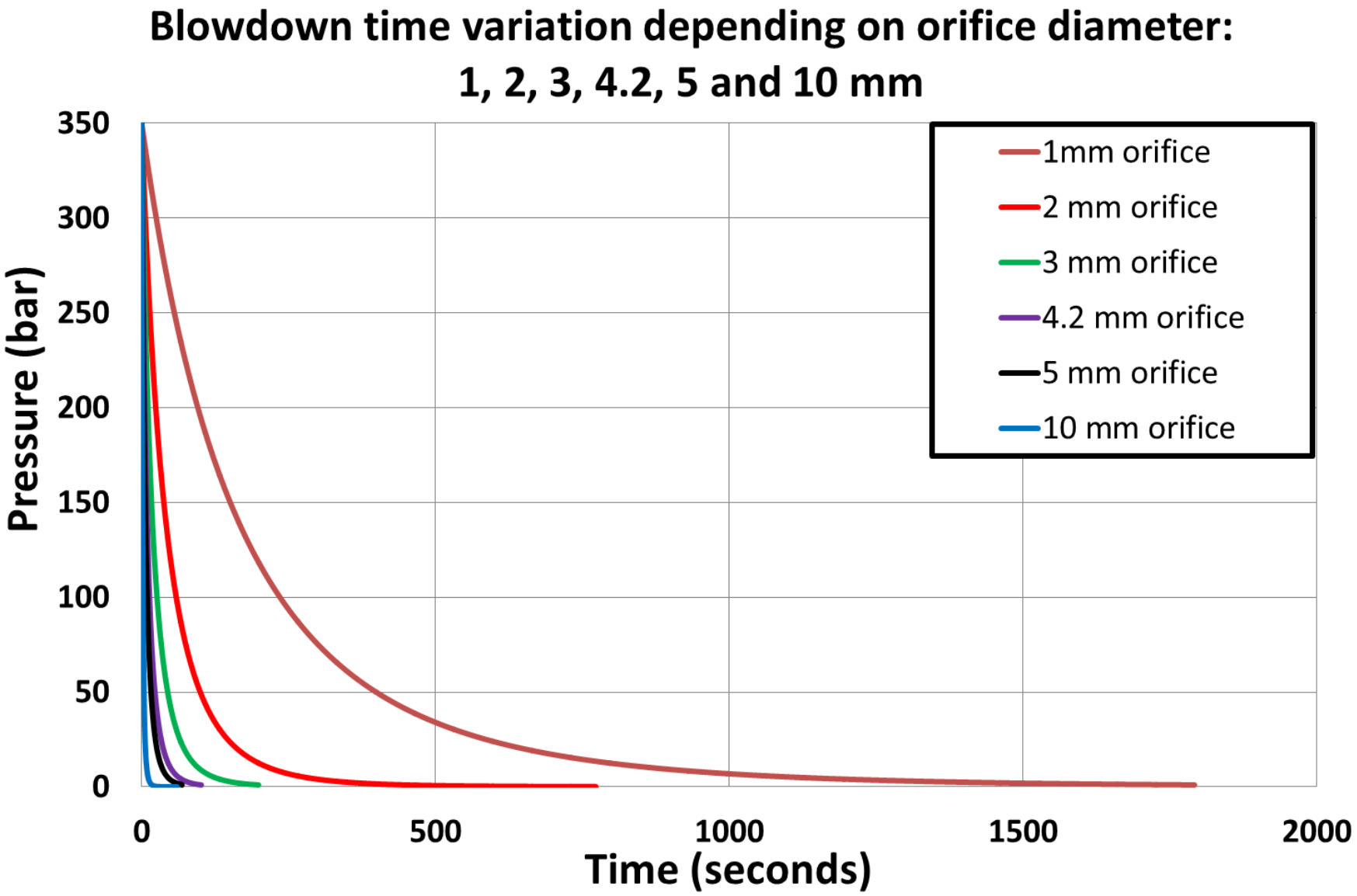


TPRD diameter (mm)	Flame length (m)	"No harm" (70^{0}C)	"Pain limit" (5 mins / 115^{0}C)	"Third degree burns" (20 s / 309^{0}C)
1	2.6	9.1	7.8	5.2
2	5.2	18.2	15.6	10.4
3	7.8	27.3	23.4	15.6
4.2	**10.9**	**38.2**	**32.8**	**21.9**
5	**13.0**	**45.5**	**39.0**	**26.0**

Blowdown time (by blowdown time)



Pressure peaking

- What if our car is parked in the garage?
  - 35 m^3 vol. (≈ garage), vent = 0.0125 m^2 (1 × typical brick)

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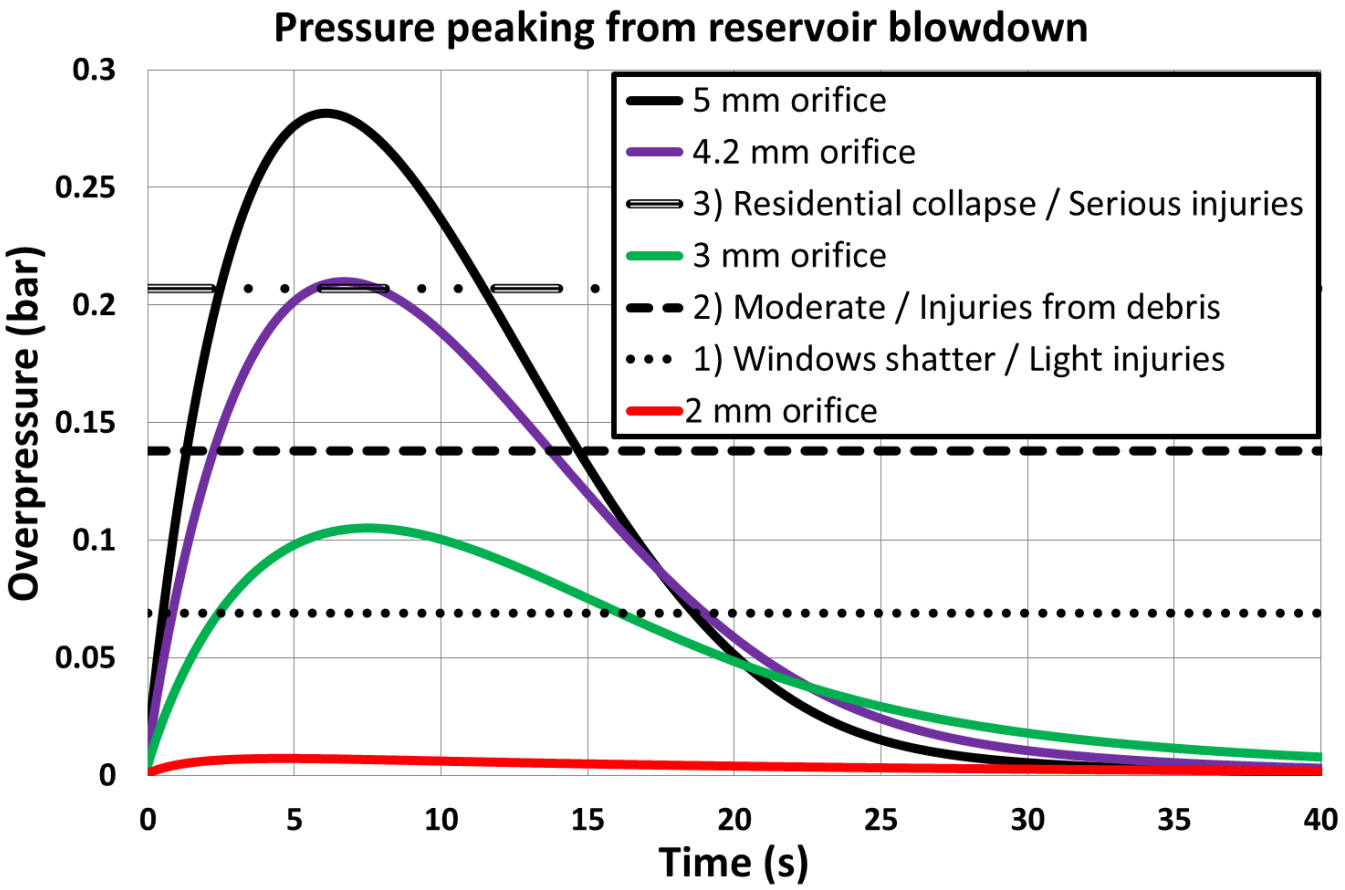
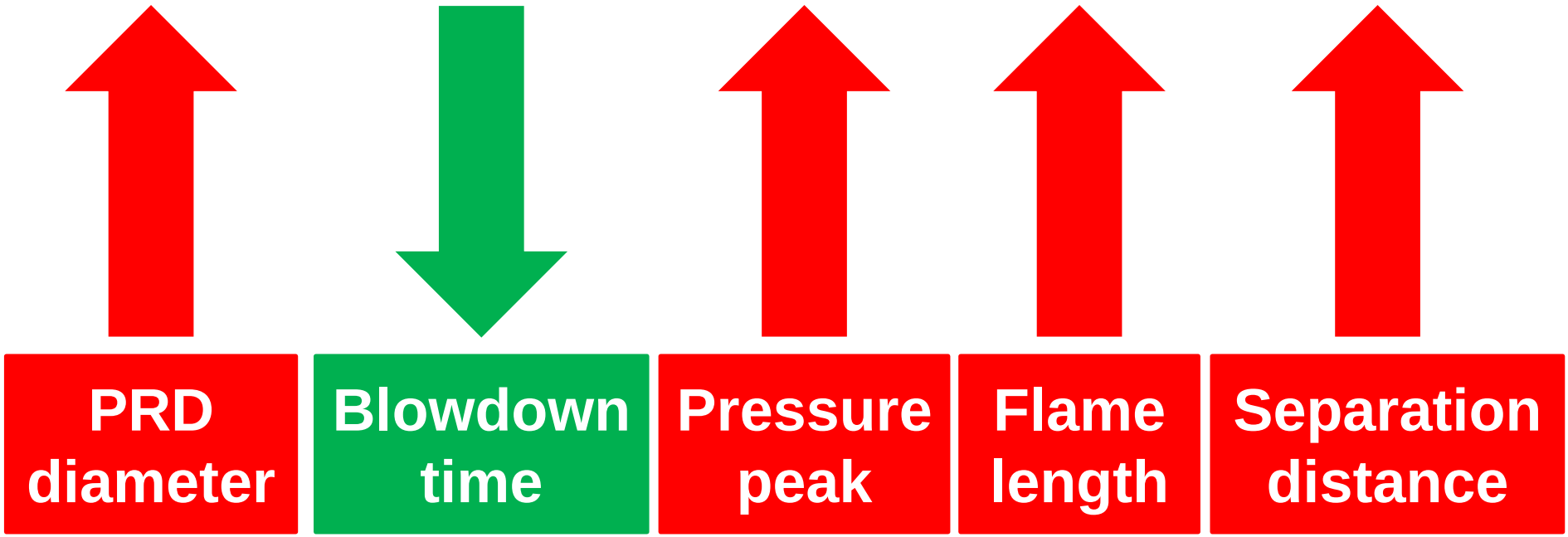


Which TPRD diameter you want?



- To select appropriate TPRD diameter: blowdown time, pressure peaking phenomenon, flame length and corresponding separation distances must all be considered in aggregate.
- Fireball from the garage and projectiles are other issues to address.

Concluding remarks

- Cyber-laboratory forms first step in creation of “one-stop-shop” for the whole FCH community.
  - Networking
  - Modelling / Simulation / Engineering tools
  - Data exploration / research / visualisation
  - User interfaces / open web services
  - Education: “Virtual knowledge centre”
- To provide open access to FCH digital resources, tools and services
- More effective collaboration between researchers
- Higher efficiency, creativity and productivity of research
- Newly developed correlations to be added as they are become available: ***Must be published and validated***.

Acknowledgment to the EC under FP7 for funding the H2FC project (www.h2fc.eu). Cyber-laboratory currently available on the H2FC website (http://h2fc.eu/cyber-laboratory)

MSc in Hydrogen Safety Engineering (distance learning course): http://www.ulster.ac.uk/elearning/programmes/view/course/10139

Fundamentals of Hydrogen Safety Engineering (free eBook, http://bookboon.com, search “hydrogen”, available since October 2012)