

Joint Summer School on Fuel Cell and Hydrogen Technology
21-25 August 2011, Viterbo, Italy

Primer

“Hydrogen properties, releases and dispersion”

Vladimir Molkov, Sile Brennan
Hydrogen Safety Engineering and Research Centre
University of Ulster

<http://hysafer.ulster.ac.uk/>

Acknowledgements

Contributions and support of:

- Colleagues from the HySAFER Centre at the University of Ulster
- Partners from the European Network of Excellence HySafe (currently International Association for Hydrogen Safety), TrainHy-Prof project and other EC-funded projects, and
- The European Commission

are gratefully appreciated.

Outline

- ❖ Introduction
- ❖ Hydrogen properties and related hazards
- ❖ Unignited releases and dispersion
 - ❖ When permeated hydrogen is safe?
 - ❖ Expanded and under-expanded jets
 - ❖ The under-expanded jet theory
 - ❖ The similarity law for concentration decay
 - ❖ Transition from momentum to buoyant jet
 - ❖ Example: hydrogen pipeline
- ❖ Pressure effects of unignited releases

Introduction



Why hydrogen?

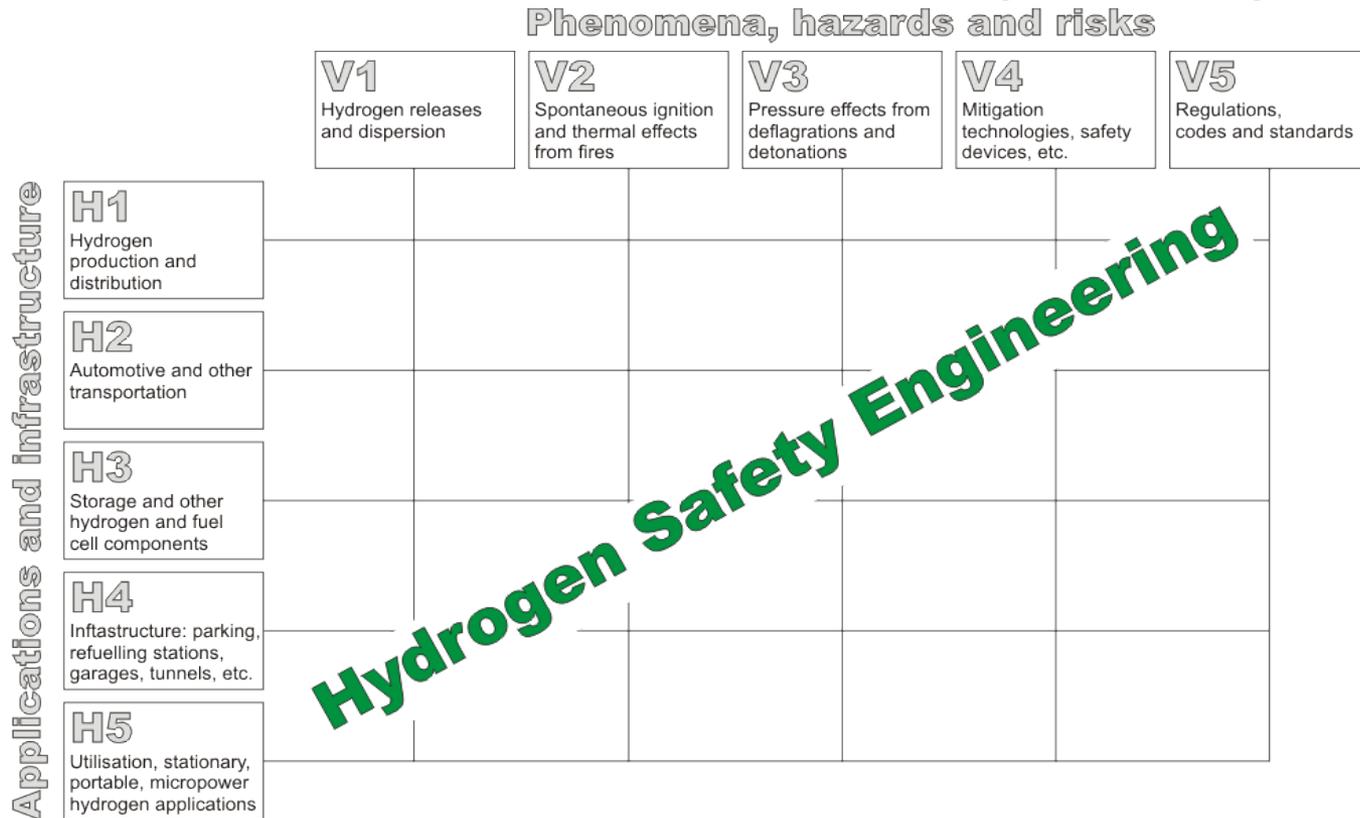
- **Fossil Fuel Reserves** (Proven reserves based on current production; source: World Coal Institute):
 - **Coal: 200 years**
 - **Gas: 70 years**
 - **Oil: 40 years**
- **Geopolitical fears:** fossil fuel depletion
- **Independence of energy supply**
- **Environment pollution:** green hydrogen (zero emission): renewable energy (wind, tide, solar, hydro) – hydrogen storage – fuel cell
- **Climate change**
- **Global market is projected to be \$8.5B by 2016.**

Hydrogen safety studies

- ❖ Initiated decades ago - result of accidents in the process industries, and were supported by safety research for nuclear power and aerospace sector.
- ❖ However, the Challenger Space Shuttle disaster (2007) and the Fukushima nuclear tragedy (2011) demonstrated that our knowledge and engineering skills to deal with hydrogen require more investment both intellectual and financial.
- ❖ Hydrogen is getting out of hands of highly trained professionals in industry and become everyday activity for public. This implies a a new safety culture, innovative safety strategies and breakthrough engineering solutions.
- ❖ It is expected that the level of safety at the consumer interface with hydrogen must be similar or exceeds that present with fossil fuel usage.
- ❖ Safety parameters of hydrogen and fuel cell products will directly define their competitiveness on the market.

Hydrogen Safety Engineering

Application of scientific and engineering principles to the protection of life, property and environment from adverse effects of incidents involving hydrogen.



World's first MSc in Hydrogen Safety Engineering

<http://campusone.ulster.ac.uk/potential/postgraduate.php?ppid=24>

Terminology (1/3)

- ❖ **Hazard** is chemical or physical condition that has the potential for causing damage to people, property and the environment.
- ❖ **Separation distance** is the minimum separation between a hazard source and an object (human, equipment or environment) which will mitigate the effect of a likely foreseeable incident and prevent a minor incident escalating into a larger incident.
- ❖ **Risk** is combination of the probability of an event and its consequence.
- ❖ **Under-expanded jet** is a jet with a pressure at the nozzle exit above the atmospheric pressure.

Terminology (2/3)

- ❖ **Flammability range** is the range of concentrations between the lower and the upper flammability limits. The lower flammable limit (LFL) is the lowest concentration of a combustible substance in a gaseous oxidizer that will propagate a flame. The upper flammable limit (UFL) is the highest concentration of a combustible substance in a gaseous oxidizer that will propagate a flame.
- ❖ **Laminar burning velocity** is the rate of flame propagation relative to the velocity of the unburned gas that is ahead of it, under stated conditions of composition, temperature, and pressure of the unburned gas.

Terminology (3/3)

- ❖ **Deflagration** and **detonation** are propagation of a combustion zone at a velocity that is respectively less and greater than the speed of sound in the unreacted mixture.
- ❖ **Stoichiometry** is the relationship between the composition of the reactants and products in a chemical reaction. Atoms are conserved in a chemical reaction, i.e. number of atoms, hydrogen, etc., in the reactant is the same as in the products. To calculate the stoichiometric composition, we assume complete combustion ($C \rightarrow CO_2$, $H \rightarrow H_2O$), $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$, $H_2 + \frac{1}{2}(O_2 + 3.76N_2) \rightarrow H_2O + 1.88N_2$
- ❖ **Equivalence ratio** is the ratio of the fuel-to-oxidizer ratio to the stoichiometric fuel-to-oxidizer ratio.

Hydrogen properties and related hazards



Hydrogen properties (1/13)

- ❖ Hydrogen is **not more dangerous or safer** compared to other fuels.
- ❖ Hydrogen safety fully depends on **how professionally it is handled** at the designed stage and afterwards.
- ❖ Hydrogen leak is difficult to detect: **colourless, odourless and tasteless** gas, **dimmiest flame** of any fuel in air
- ❖ **High pressures** (humans, equipment, structures): hydrogen systems are used at pressures up to 100 MPa
- ❖ **Low temperatures** (cold burns): down to -253°C (liquefied hydrogen)

Hydrogen properties (2/13)

- ❖ Burns in clean atmosphere with “invisible” flame.
- ❖ More **prone to deflagration-to-detonation transition** compared to most of flammable gases.
- ❖ The smallest **minimum ignition energy (MIE)** of 0.019 mJ.
- ❖ The narrowest **minimum experimental safety gap (MESG)** of 0.08 mm to prevent flame propagation out of a shell, composed of two parts, through the gap between two flanges.
- ❖ The main hydrogen safety asset, i.e. its highest on Earth **buoyancy**, confers the ability to rapidly flow out of an incident scene, and mix with the ambient air to a safe level below the LFL (4% v/v in air).

Hydrogen properties (3/13)

- ❖ The **energy density** of hydrogen is 132.5 MJ/kg. This is approximately 2.5 times larger than of natural gas (and other fossil fuels).
- ❖ On the other hand, for the same volumetric leak rate the energy content of a hydrogen leak is smaller than that of hydrocarbons (lowest density).
- ❖ The **lower heating value** of hydrogen is 242 kJ/mol and the **higher heating value** is 286 kJ/mol. The difference of about 16% is due to the heat of condensation of water vapour, and this value is larger compared to other gases.
- ❖ The **specific heat ratio** of hydrogen at NTP (293.15 K and 101.325 kPa) is 1.405.

Hydrogen properties (4/13)

- ❖ Hydrogen has a somewhat higher **adiabatic flame temperature** of stoichiometric mixture in air of 2403 K.
- ❖ The **laminar burning velocity** of a stoichiometric hydrogen-air mixture can be calculated as an experimental propagation velocity, observed by a schlieren system, divided by the **expansion coefficient** of combustion products $E_i=7.2$, and is accepted in HySAFER numerical studies as 1.91 m/s (Lamoureaux et al., 2002).
- ❖ This laminar burning velocity is far greater compared to most of hydrocarbons when velocities are in the range 0.30-0.45 m/s.

Hydrogen properties (5/13)

- ❖ It is worth noting that the **maximum burning velocity** for hydrogen-air mixture is reached not at stoichiometric mixture of 29.5% by volume yet in a rich mixture with concentration of hydrogen in air 40.1%, when it is 2.44 m/s (Lamoureaux et al., 2002).
- ❖ This is due to the high molecular diffusivity of hydrogen, with the **diffusion coefficient** equal to $6.1\text{E-}05\text{ m}^2/\text{s}$.
- ❖ Thus, the maximum burning velocity for a hydrogen-air premixed flame occurs at an **equivalence ratio 1.8** while for hydrocarbon-air flames it occurs at around 1.1.

Hydrogen properties (6/13)

- ❖ The **flammability range** of hydrogen, on the one hand, is wider compared to most hydrocarbons, i.e. 4% to 75% by volume in air at NTP.
- ❖ The flammability range expands with temperature, e.g. the lower flammability limit (upward propagation) drops from 4% at NTP to 3% at 100°C.
- ❖ The LFL of hydrogen depends on a direction of flame propagation. In initially quiescent mixture LFL is:
 - ❖ 4% by volume (NTP) for **upward** propagation,
 - ❖ 7.2% for **horizontally** propagating flames, and
 - ❖ 8.5-9.5% for **downward** and spherically propagating flames (Coward and Jones, US Bureau of Mines, 1952).

Hydrogen properties (7/13)

- ❖ Upward flame propagation at LFL of 4% is in a form of separate “bubbles” with unburnt mixture in between.
- ❖ This explains why burning of quiescent 4% hydrogen-air mixture in a closed vessel can generate negligible in a practical sense overpressure.
- ❖ It is worth noting that a quiescent hydrogen-air mixture in the range of concentration **4-7.1% could burn practically without overpressure** for a number of scenarios, e.g. if ignited at the top of an enclosure (in such conditions it cannot propagate flame in any direction and thus no heat release accompanied by pressure build up can be observed).

Hydrogen properties (8/13)

- ❖ On the other hand, the lower flammability limit of hydrogen is high compared to most hydrocarbons.
- ❖ Near-stoichiometric hydrogen concentration of hydrogen 29.5% by volume in air is greatly higher compared to only a few percent for hydrocarbons.
- ❖ Moreover, at the lower flammability limit the ignition energy requirement of hydrogen is similar to that of methane, and weak ignition sources such as electrical equipment sparks, electrostatic sparks or sparks from striking objects typically involve more energy than is required to ignite these flammable mixtures

Hydrogen properties (9/13)

- ❖ Compared to other fuels H₂ is the most prone to **spontaneous ignition** during sudden releases to air by so-called diffusion mechanism, when heated by a shock air mixes with cold hydrogen at the contact surface between these two gases and chemical reactions can be initiated when critical conditions are reached. Hydrogen sudden releases into piping with air can be spontaneously ignited at about 2 MPa.
- ❖ Lowest autoignition temperature of any fuel ignited by a **heated air jet** (640°C).
- ❖ On the other hand, the **standard auto-ignition temperature** (heated flask) of hydrogen in air is above 520°C that is higher than for hydrocarbons.

Hydrogen properties (10/13)

- ❖ Hydrogen is essentially an **insulator** in both gaseous and liquid phases. Only above some critical “breakdown” voltage, where ionization occurs, does it become an electrical conductor.
- ❖ When high velocity hydrogen flow accompanies high-pressure vessel blowdown this property can potentially be responsible for the generation of **static electrical charge by triboelectricity**. The probability of hydrogen ignition by this mechanism increases with increase of the blowdown time.

Hydrogen properties (11/13)

- ❖ Detonation is the worst case scenario for hydrogen accident. The **detonability range** of hydrogen in air is 11-59% by volume. This is narrower and within the flammability range of 4-75%.
- ❖ The detonability limits are not fundamental characteristics of the mixture as they strongly depend on size of an experimental set up.
- ❖ Indeed, a diameter of the tube, where detonation can propagate, should be of the order of a detonation cell size. A detonation cell size increases with approaching the detonability limits. Thus, the larger is the scale of an experimental apparatus the smaller is the lower detonability limit (the larger is the UDL).

Hydrogen properties (12/13)

- ❖ The detonability limits of hydrogen-air mixture of the same concentration expand with the scale of a flammable cloud.
- ❖ This explains the difference between the lower detonability limit of hydrogen 11% by volume reported in (EIHP2 report, 2001) and the underestimated value of 18% published in standard ISO/TR 15916:2004.
- ❖ Experimental values of **detonation cell size** for a stoichiometric hydrogen-air mixture are 1.1-2.1 cm.
- ❖ The **run-up distance** for transition from deflagration to detonation (DDT) in stoichiometric hydrogen-air mixture has L/D ratio of approximately 100.

Hydrogen properties (13/13)

- ❖ The main safety asset of hydrogen is buoyancy as underlined above. Indeed, hydrogen has a density of 0.0838 kg/m^3 (NTP). This is far lower than air which has a density of 1.205 kg/m^3 .
- ❖ The unwanted consequences of hydrogen releases into the open atmosphere, and in partially confined geometries, where no conditions of hydrogen accumulating, are drastically reduced by buoyancy.
- ❖ Contrary, heavier hydrocarbons are able to form a huge combustible cloud, as in disastrous Flixborough (1974) and Buncefield (2005) explosions.
- ❖ In many practical situations hydrocarbons may pose stronger fire and explosion hazards than hydrogen.

When permeated hydrogen dispersion in garage is safe?

3

Permeation (1/5)

- ❖ The permeation rate of hydrogen through a particular material depends on **temperature, internal pressure and membrane thickness** (mol/s/m²):

$$J = P_0 \exp(-E_0 / RT) \frac{\sqrt{P_r}}{l}$$

- ❖ Three main phenomena drive the dispersion of permeated hydrogen: buoyancy, diffusion, and natural ventilation.
- ❖ **The perfect mixing equation** for concentration can be used to calculate the hydrogen leak rate Q_g

$$C_{\%} = \frac{100 \cdot Q_g}{Q_a + Q_g}$$

Permeation (2/5)

- ❖ The maximum allowable permeation rate is

$$Q_{perm}^{max} = \frac{Q_a \cdot C_{\%}}{100 - C_{\%}} \cdot \frac{1}{V \cdot f_a \cdot f_t} [NmL / hr / L]$$

where Q_a – air flow, NmL/hr, V – water capacity of hydrogen storage, L; f_a – aging factor, taken to be 2, for unknown aging effects; f_t – test temperature factor (3.5 at test temperature 20°C, 4.7 – 15°C)

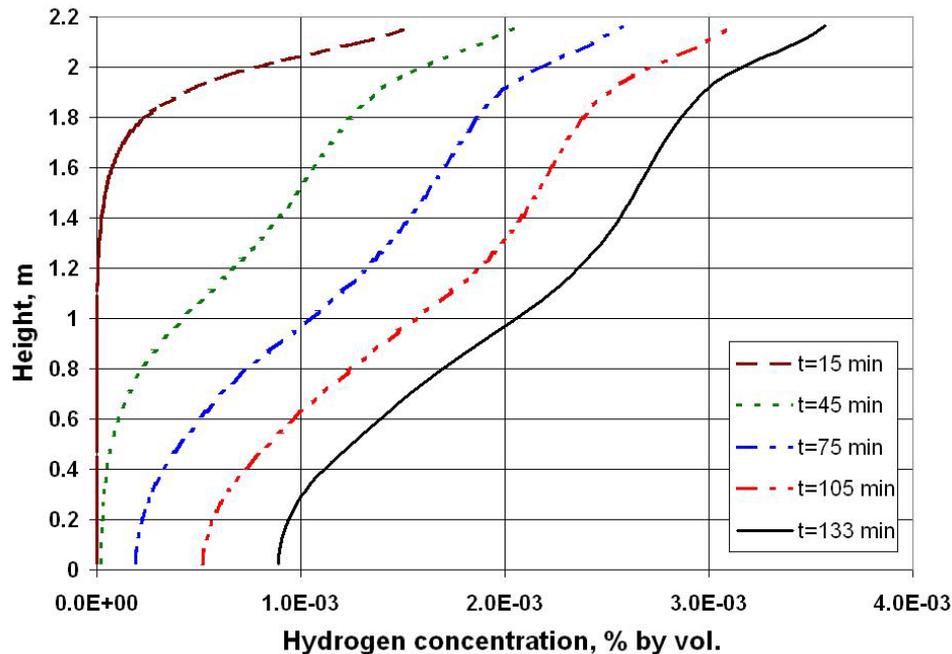
- ❖ **Does dispersion of permeated hydrogen leads to perfect mixing in garage?** Permeation-induced release of hydrogen *is different compared to plumes and jets: hydrogen releases in very small amounts equally along the surface of a storage tank.*

Permeation (3/5)

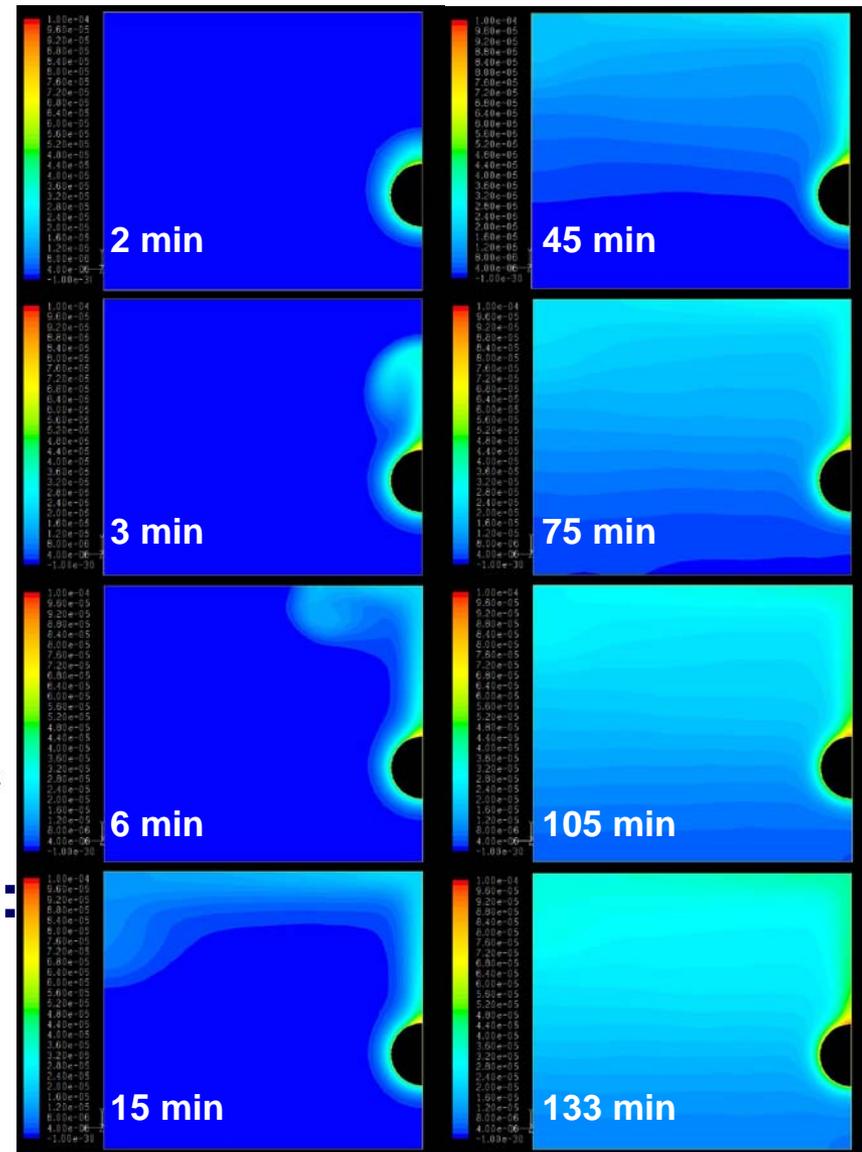
- Modelling approach: **volumetric release of hydrogen in a thin layer around the tank surface** of 1.87 m². No artificial source with a mass fraction $Y_{H_2}=1$ at “release orifice” (there is no layer $Y_{H_2}=1$ on the tank’s surface). Permeation rate 1.14 NmL/hr/L.
- Typical garage $L \times W \times H = 5 \times 3 \times 2.2$ m ($V = 33$ m³). Tank $L = 0.672$ m, $D = 0.505$ m, hemisphere at each end ($V = 0.2$ m³). Floor clearance is 0.5 m. $T = 298$ K.
- Time to reach LFL of 4% in the **closed** garage with chosen tank and permeation rate will be **240 days**.
- Time for hydrogen diffusion through the height of the garage is H^2/D_{H_2} (at 298 K as $D_{H_2} = 7.79 \cdot 10^{-5}$ m²/s). Indeed, $H^2/D_{H_2} = 2.2^2 / 7.79 \cdot 10^{-5} = 62051$ s or **0.7 days**.

Permeation (4/5)

**CFD: negligible stratification
(no areas of 100% hydrogen)**



**Max concentration at 133 min:
tank top - 8.2×10^{-3} % by vol.;
ceiling - 3.5×10^{-3} % by vol.**



Permeation (5/5)

- ❖ Thus, with **homogeneously dispersed permeated hydrogen**, at reasonable minimum natural ventilation rate of 0.03 ac/hr, at reasonable maximum prolonged material temperature of 55°C (test temperature factor 4.7 for 15°C), with aging factor 2, the maximum hydrogen concentration will not be above 1% by vol if **permeation rate for new tank is below 6 NmL/hr/L (15°C), or 8 NmL/hr/L (20°C).**

For comparison:

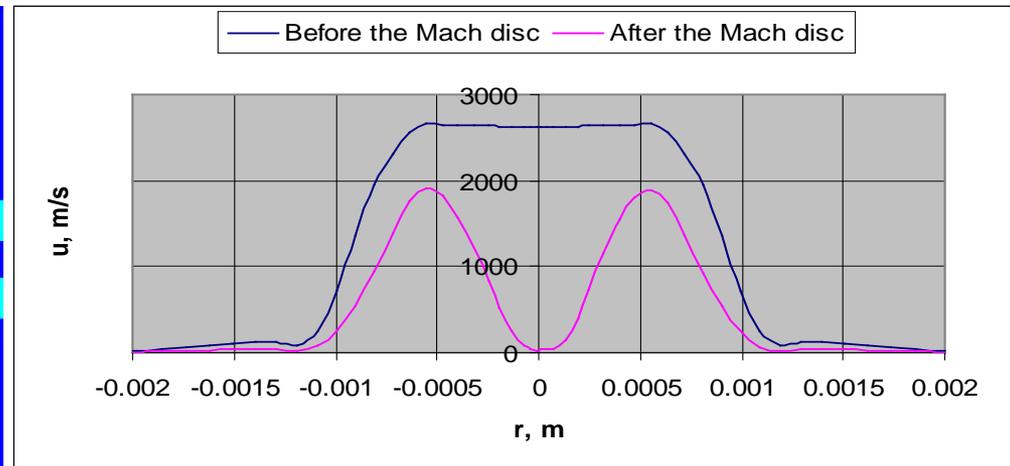
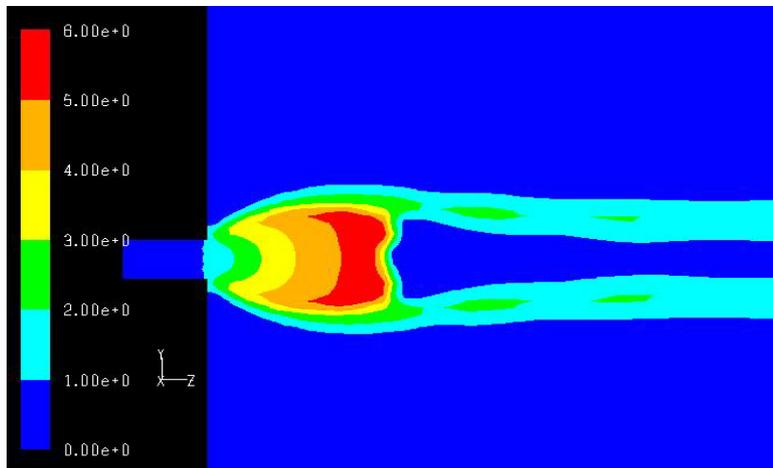
- ❖ Japan Automotive Research Institute: **5 NmL/hr/L (15°C).**
- ❖ Society of Automotive Engineers J2579, end of life, 55°C:
150 NmL/min/vehicle
(HySafe equivalent figure would be **90 NmL/min/vehicle**)
- ❖ ISO/TS15869:2009 at end of life (20°C):
75 NmL/min/container
- ❖ **With this level of permeation rate the hydrogen dispersion in typical garage is not a problem!**

Expanded and under-expanded jets



Expanded and under-expanded jets

- ❖ **Expanded jet** – pressure at the nozzle end is atmospheric (storage pressure below 1.9 bar abs.).
- ❖ **Under-expanded jet** - pressure at the end of a nozzle has not fully dropped to the atmospheric pressure. The exit velocity remains locally sonic (choked flow in the nozzle). **Non-uniform velocity!**



Jets: subsonic, sonic, supersonic

❖ Speed of sound is

$$C = \sqrt{\gamma \frac{P}{\rho}} = \sqrt{\gamma \frac{RT}{M}}$$

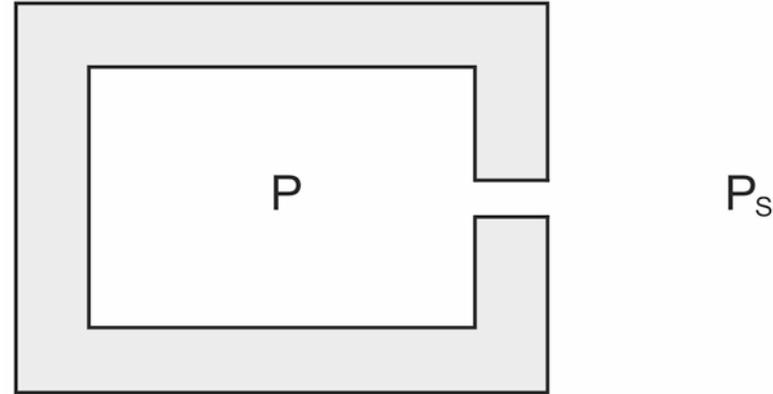
❖ Subsonic flow: velocity $U < C$

$$\frac{P_s}{P} \geq \left(\frac{2}{\gamma + 1} \right)^{\gamma/(\gamma-1)} = \frac{1}{1.89}$$

$$\dot{m} = \mu A \left\{ \left(\frac{2\gamma}{\gamma-1} \right) P \rho \left[\left(\frac{P_s}{P} \right)^{2/\gamma} - \left(\frac{P_s}{P} \right)^{(y+1)/\gamma} \right] \right\}^{1/2}$$

❖ Sonic flow: velocity $U = C$, choked flow ($M = U/C = 1$)

❖ Supersonic flow: velocity is larger than the speed of sound ($U > C$)



Jets: subsonic, sonic, supersonic

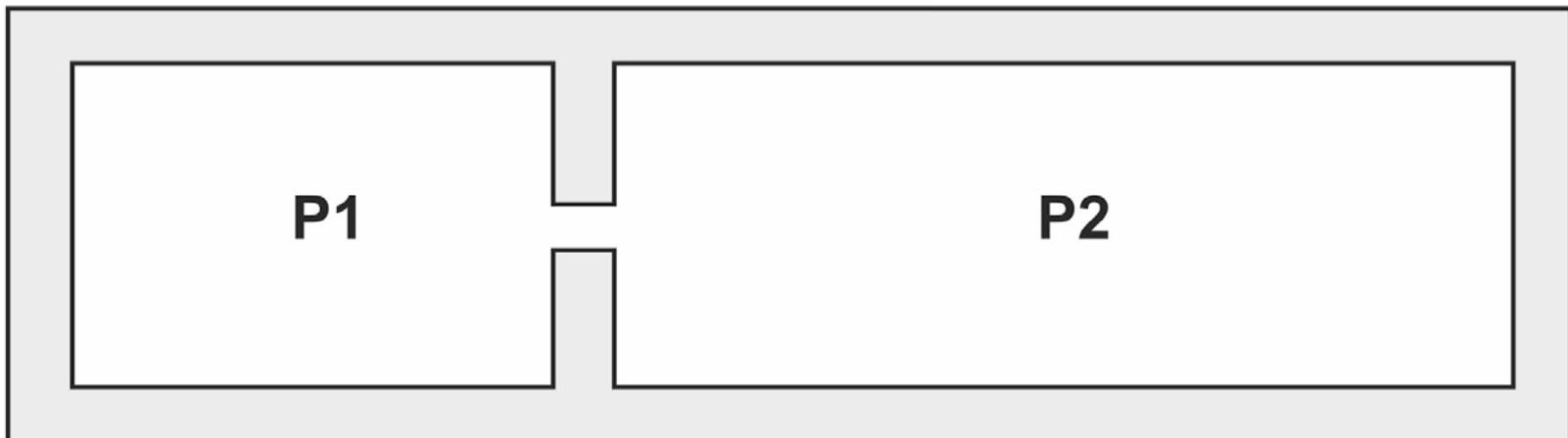
J. Fluid Mech., 392, pp.129-153

❖ Subsonic matched jets:

ratios of pressure in high-pressure and low-pressure chambers is $P1/P2=1-4.1$ (theoretical ratio $P1/P2=1.9$, ...losses...?)

❖ Sonic under-expanded jets: $P1/P2=4.1-41.2$

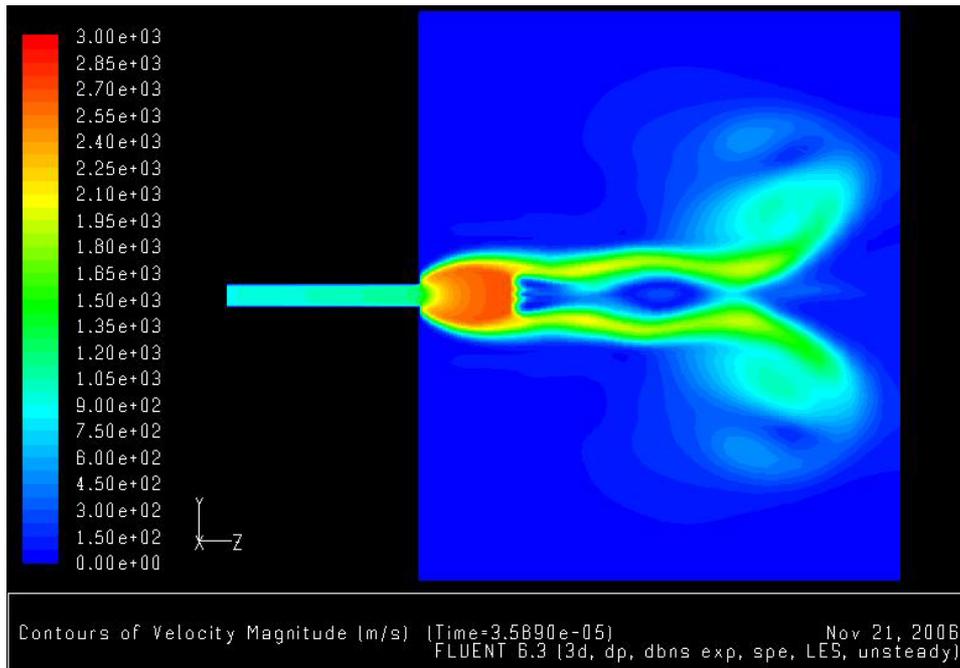
❖ Supersonic under-expanded jets: $P1/P2 > 41.2$



LES of under-expanded jet

Release of hydrogen to atmosphere:

- Tank pressure 161 atm
- Nozzle diameter 0.25 mm
- Mass flow rate 0.46 g/s



Simulations:

- Velocity
- H₂ mole fraction
- Temperature

Under-expanded jet theory



Notional nozzle theories

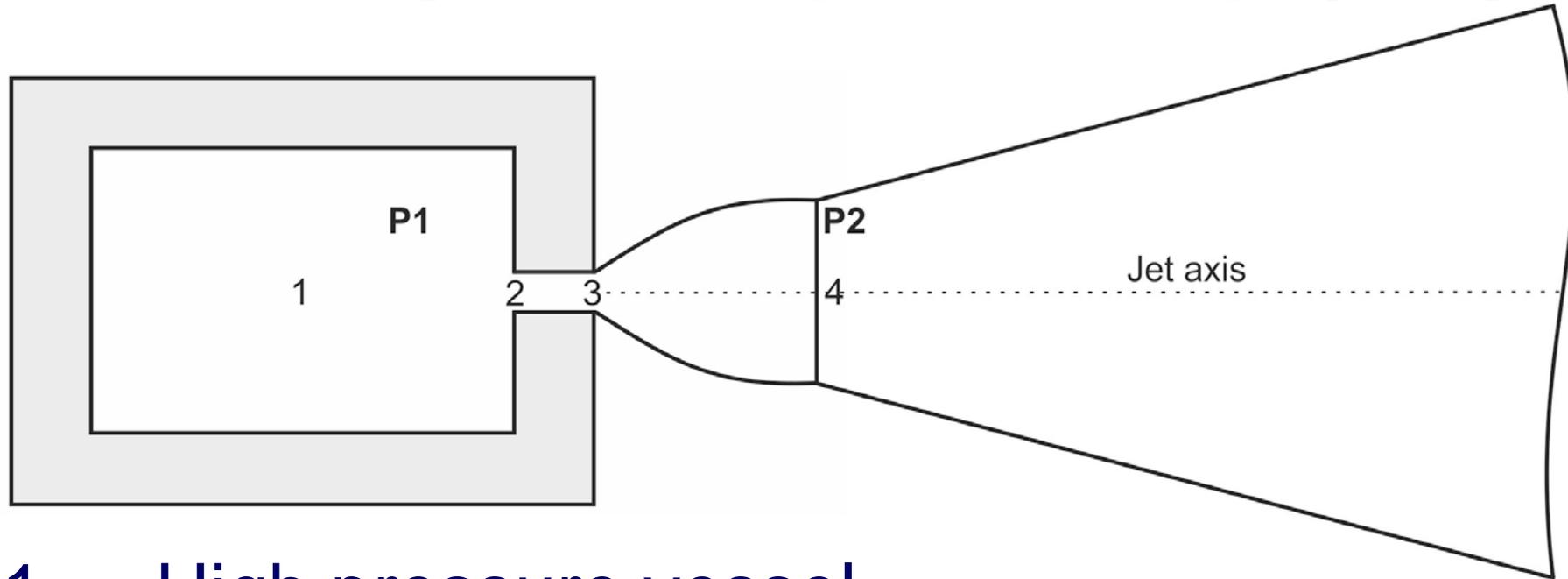
- ❖ Former theories by Birch et al. (1984, 1987), Evan and Moodie (1986) based on ideal gas equation can not be applied at pressures above 100 bar.
- ❖ The Abel-Noble equation is applied (at 700 bar the ideal gas law results in 50% higher “released mass”).

$$P = \frac{\rho RT}{(1 - b\rho)M}$$

co-volume constant $b = 7.69\text{E-}03 \text{ m}^3/\text{kg}$.

- ❖ Schefer et al. (2007) the first notional nozzle theory accounting for non-ideal behaviour of H₂.
Mass and momentum conservation – supersonic flow at the notional nozzle.

Under-expanded jet theory (1/2)



1 High pressure vessel

2 Entrance to nozzle

3 Exit from nozzle

4 Notional nozzle (3-4: no entrainment)

P1 Storage pressure

P2 Atmospheric pressure after jet expansion

Under-expanded jet theory (2/2)

Details of the theory:

Molkov V, Makarov D, Bragin M. Physics and modelling of under-expanded jets and hydrogen dispersion in atmosphere, In: Physics of extreme state of matter 2009, Chernogolovka, 2009, 143-145.

$\rho_1 = \frac{p_1}{bp_1 + R_{H2}T_1}$	$u_4 = a_4 = \sqrt{\gamma R_{H2}T_4}$ Assumption
$c_p T_1 = c_p T_3 + \frac{u_3^2}{2}$	$\rho_4 = \frac{p_4}{R_{H2}T_4}$
$\rho_3 = \frac{p_3}{bp_3 + R_{H2}T_3}$	$c_p T_3 + \frac{u_3^2}{2} = c_p T_4 + \frac{u_4^2}{2}$
$u_3^2 = a_3^2 = \frac{\mathcal{P}_3}{\rho_3(1 - b\rho_3)}$	$\rho_3 u_3 A_3 = \rho_4 u_4 A_4$
$p_1 \left(\frac{1}{\rho_1} - b \right)^\gamma = p_3 \left(\frac{1}{\rho_3} - b \right)^\gamma$	Unknown parameters: $\rho_1, \rho_3, u_3, T_3, p_3, \rho_4, u_4, T_4, A_4$. Know parameters: p_1, T_1, A_3, p_4 and constants c_p, R_{H2}, b, γ .

The similarity law for concentration decay



- Study of entrainment into jets:
 - high Reynolds numbers,
 - distances with large length to diameter L/D ratio
- Dimensional analysis:

the mass flow rate, including entrained air, at right angle to the jet axis is **proportional to distance x** (M_0 - momentum flux of the jet at orifice)

$$m(x) = K_1 M_0^{1/2} \rho_s^{1/2} x$$

$$M_0 = \rho_N U^2 \pi D^2 / 4$$

$K_1=0.282$ irrespective of the density ratio

- Experimentally proved that this equation holds for non-uniform density **provided that buoyancy effects are negligible**. Experimental data obey the relation (tested by isothermal injection of hydrogen)

$$\frac{m(x)}{m_N} = 0.32 \frac{x}{D} \sqrt{\frac{\rho_S}{\rho_N}}$$

- Reciprocal to the left-hand side of the previous equation by Ricou and Spalding (1961) is a **fuel mass fraction averaged through the jet cross-section**

$$C_{av} = 3.1 \sqrt{\frac{\rho_N}{\rho_S}} \frac{D}{x}$$

Expanded jets: 1957-1980

- ❖ 1957, Thring et al.:

$$C_{ax} = 5.0 \sqrt{\frac{\rho_N}{\rho_S} \frac{D}{x}} \sqrt{\frac{T_S}{T_N}}$$

- ❖ 1961, Ricou and Spalding (**averaged** fuel mass fraction):

$$C_{av} = 3.1 \sqrt{\frac{\rho_N}{\rho_S} \frac{D}{x}}$$

- ❖ 1980, Chen and Rodi (**axial** fuel mass fraction):

$$C_{ax} = 5.4 \sqrt{\frac{\rho_N}{\rho_S} \frac{D}{x}}$$

$$x = 5.4 \sqrt{\frac{\rho_N}{\rho_S} \frac{D}{C_{ax}}}$$

- ❖ **Conclusion:**

Flammable envelope size, i.e. distance to LFL of 4% by volume, increases proportional to orifice diameter.

Under-expanded jets: 1984-1987

- ❖ **Birch et al., 1984.** Natural gas (2-70 bar).
Notional nozzle diameter

$$D_{eff} \propto D \sqrt{p_R / p_S}$$

Mean **volumetric** fraction (subcritical natural gas virtual origin: $x_0 = -3.6$; supercritical: $x_0 = -0.1$)

$$C_{ax} = 4.9 \sqrt{\frac{\rho_S}{\rho_N} \frac{D_{eff}}{x + x_0}}$$

- ❖ **Birch et al., 1987,** for relatively high pressures ($x_0 = 0.6D$ being small):

$$C_{ax} = 5.4 \sqrt{\frac{\rho_S}{\rho_N} \frac{D_{eff}}{x}} \quad \text{with} \quad \frac{D_{eff}}{D} = \sqrt{\frac{p_R}{p_S} \left(\frac{2}{\gamma + 1} \right)^{1/(\gamma-1)} \frac{1}{(\gamma + 1)}}$$

Expanded VS under-expanded

- ❖ The similarity law - **expanded** jets
(1980, Chen and Rodi)

$$C_{ax}^m = 5.4 \sqrt{\frac{\rho_N}{\rho_S}} \frac{D}{x}$$

- ❖ The similarity law – **under-expanded** jets
(1987, Birch et al)

$$C_{ax}^V = 5.4 \sqrt{\frac{\rho_S}{\rho_N}} \frac{D_{eff}}{x}$$

Three contradictions:

- ❖ Volume fraction (1987) instead of mass fraction
- ❖ Density ratio is reciprocal
- ❖ Notional nozzle (1987) instead of real nozzle

How to calculate decay in jets?

The similarity law - **solution**

- ❖ The original form of the similarity law (**expanded jets**) by Chen and Rodi (1980)

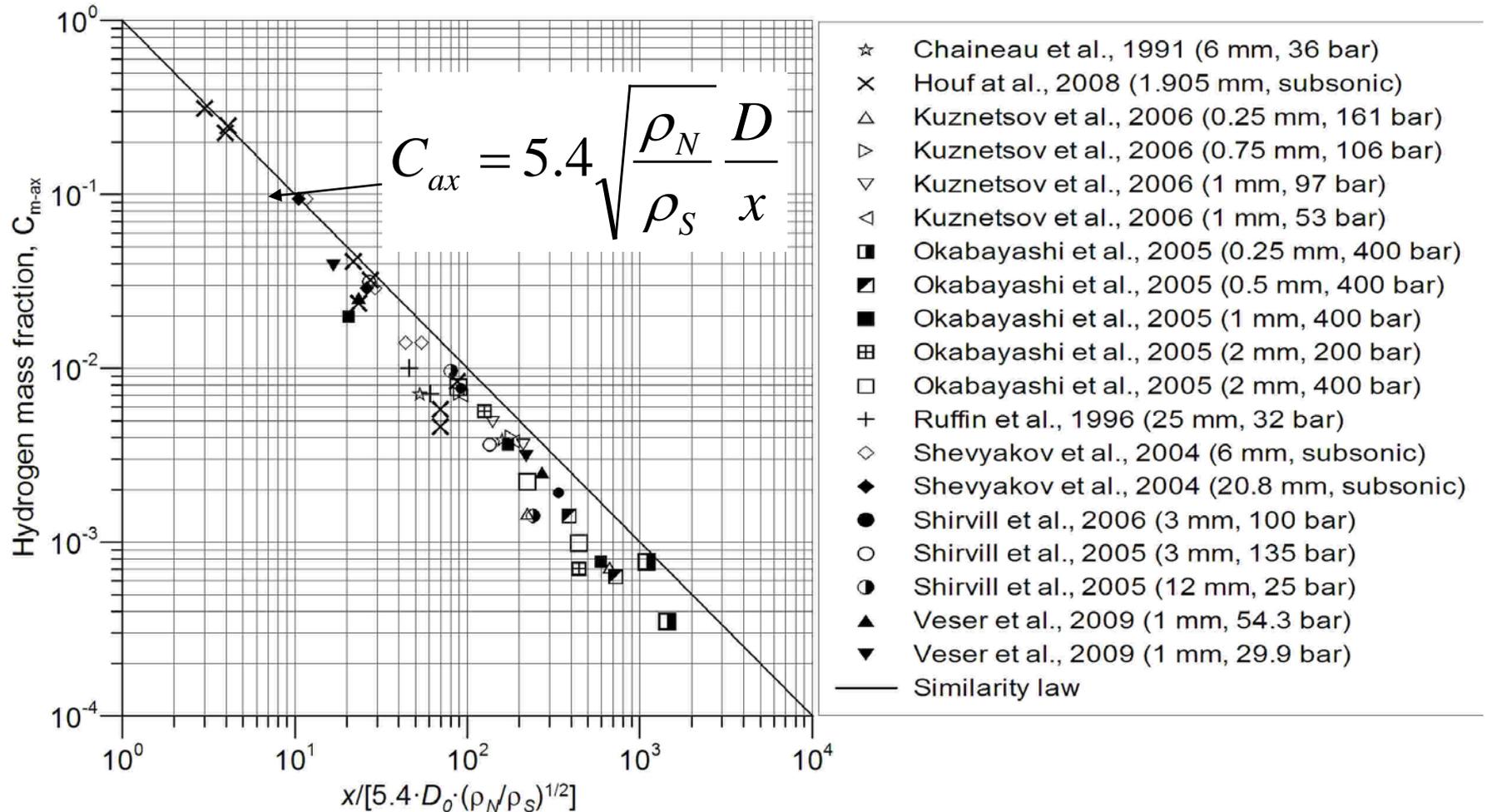
$$C_{ax}^m = 5.4 \sqrt{\frac{\rho_N}{\rho_S}} \frac{D}{x}$$

with **the only “unknown”** parameter - **density in the nozzle** (physical nozzle size is applied).

- ❖ “Unknown” density is calculated by an **under-expanded jet theory*** developed at the University of Ulster (ρ_N affects the flammable envelope size of 4% by vol. i.e. 0.00288 mass fraction; 0.00141 - 2%, 0.0007 - 1%).

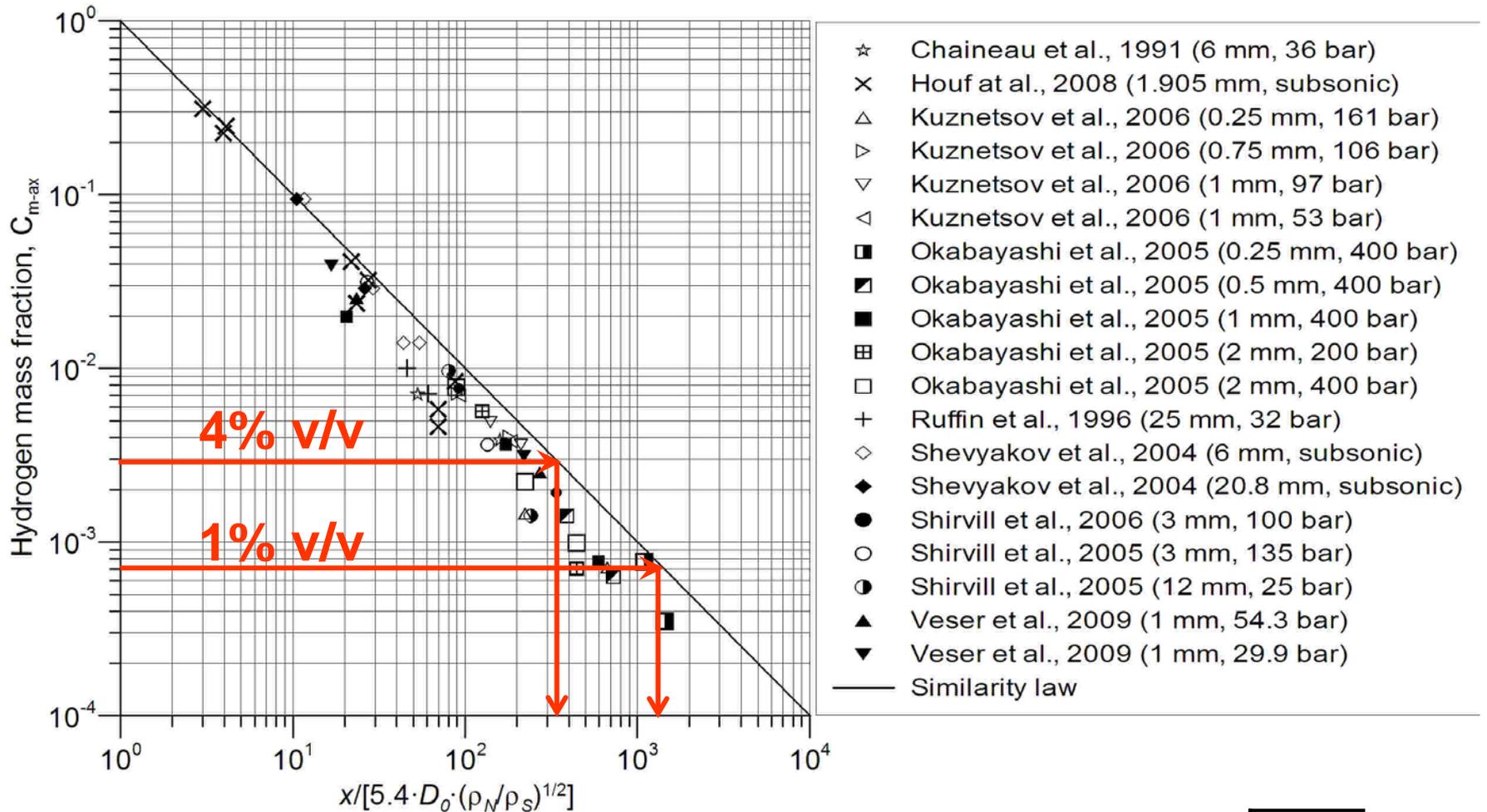
The similarity law - validation

53 points, $P < 40$ MPa, $T > 80$ K (cold jets), $D = 0.25$ -25 mm, 1-86.6%, $x/D = 4$ -28580 (before < 170), $Re = 927$ - 7.1×10^6



The similarity law is conservative to tests - effect of losses

Separation distance



Distance to 4% by volume: $x = 1709 \cdot \sqrt{\rho_N} \cdot D$

Useful information

- ❖ The mass fraction (C_M) can be calculated by the volumetric (mole) fraction (C_V)

$$1/C_M = 1 + (1/C_V - 1)M_S/M_N,$$

where M_S and M_N are molecular mass of surrounding gas and nozzle gas respectively.

- ❖ Mass fraction 0.0288 corresponds to 30% of hydrogen by volume in air, 0.00639 - 8.5%, 0.00288 - 4%, 0.00141 - 2%, 0.0007 - 1%.

- ❖ The ratio of distance to diameter (x/D) is equal for a number of hydrogen concentrations (with $\rho_S/\rho_N = 14.38$ ($\rho_N = 0.0838$, $\rho_S = 1.205$ in the case of **fully expanded flow in a real nozzle**):

49 $x/D_{30\%} = 49.1$; $x/D_{4\%} = 491$; $x/D_{2\%} = 1003$; $x/D_{1\%} = 2019$.

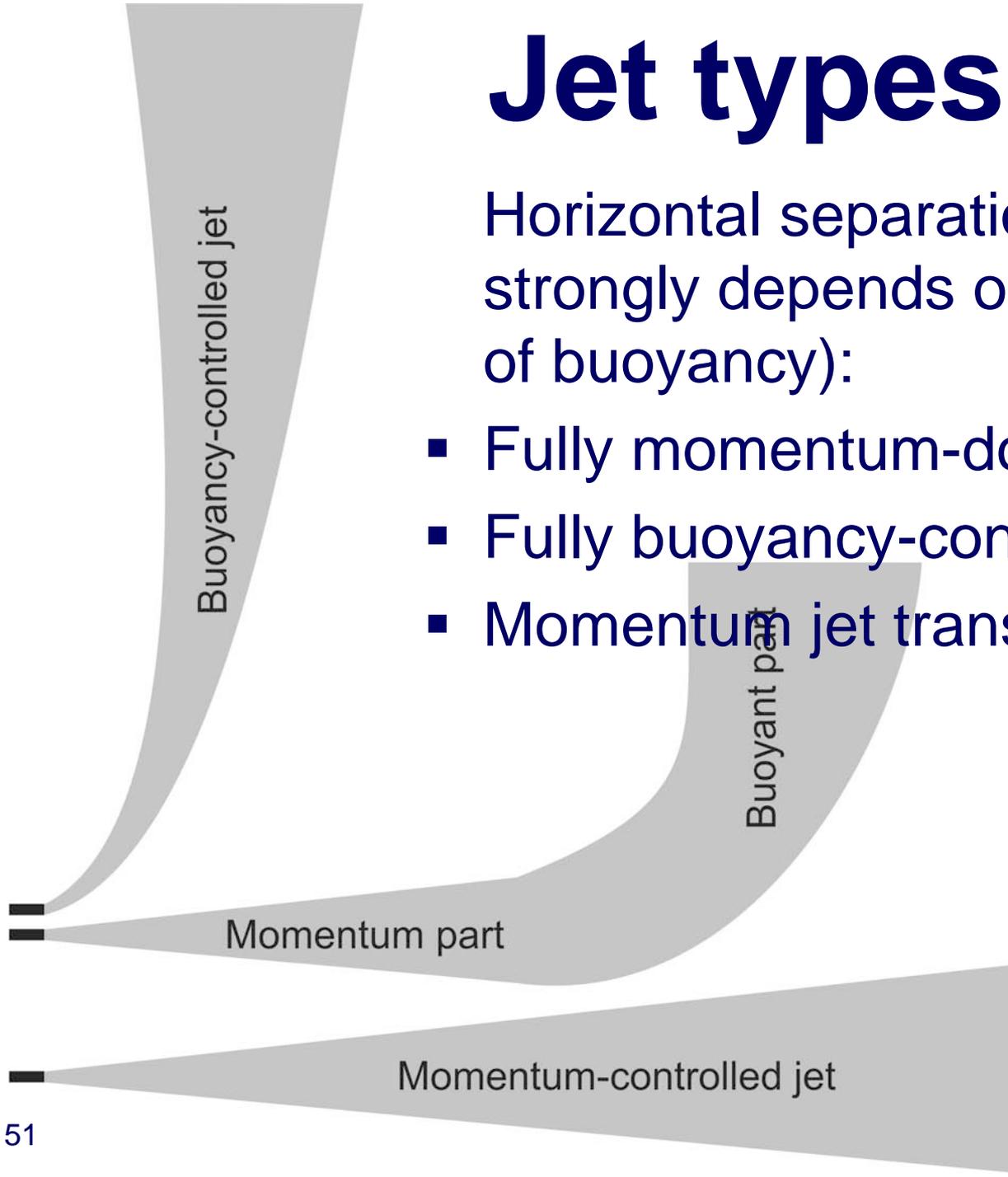
Momentum- and buoyancy- controlled jets



Jet types

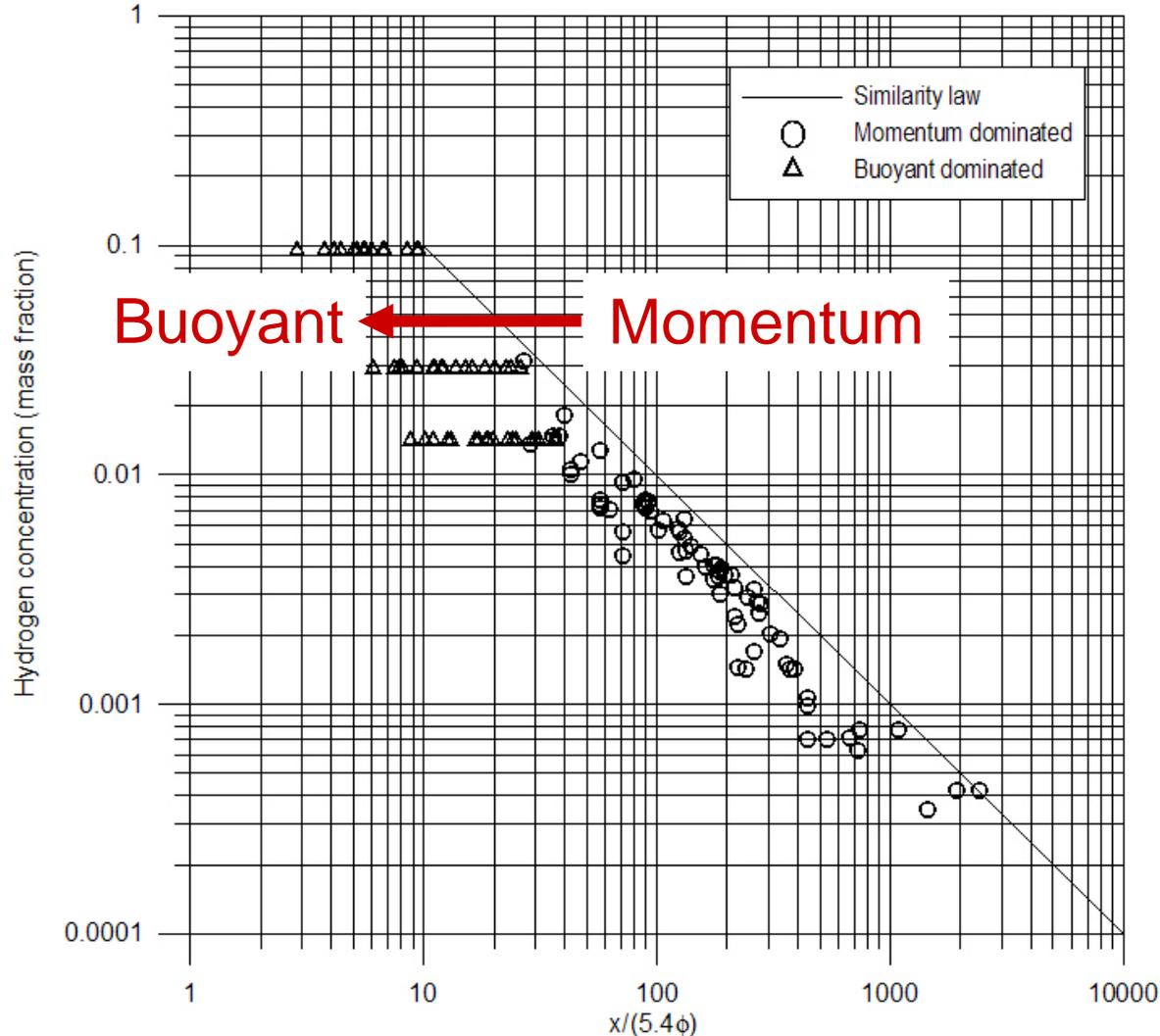
Horizontal separation distance strongly depends on jet type (effect of buoyancy):

- Fully momentum-dominated jet
- Fully buoyancy-controlled jet
- Momentum jet transits to buoyant



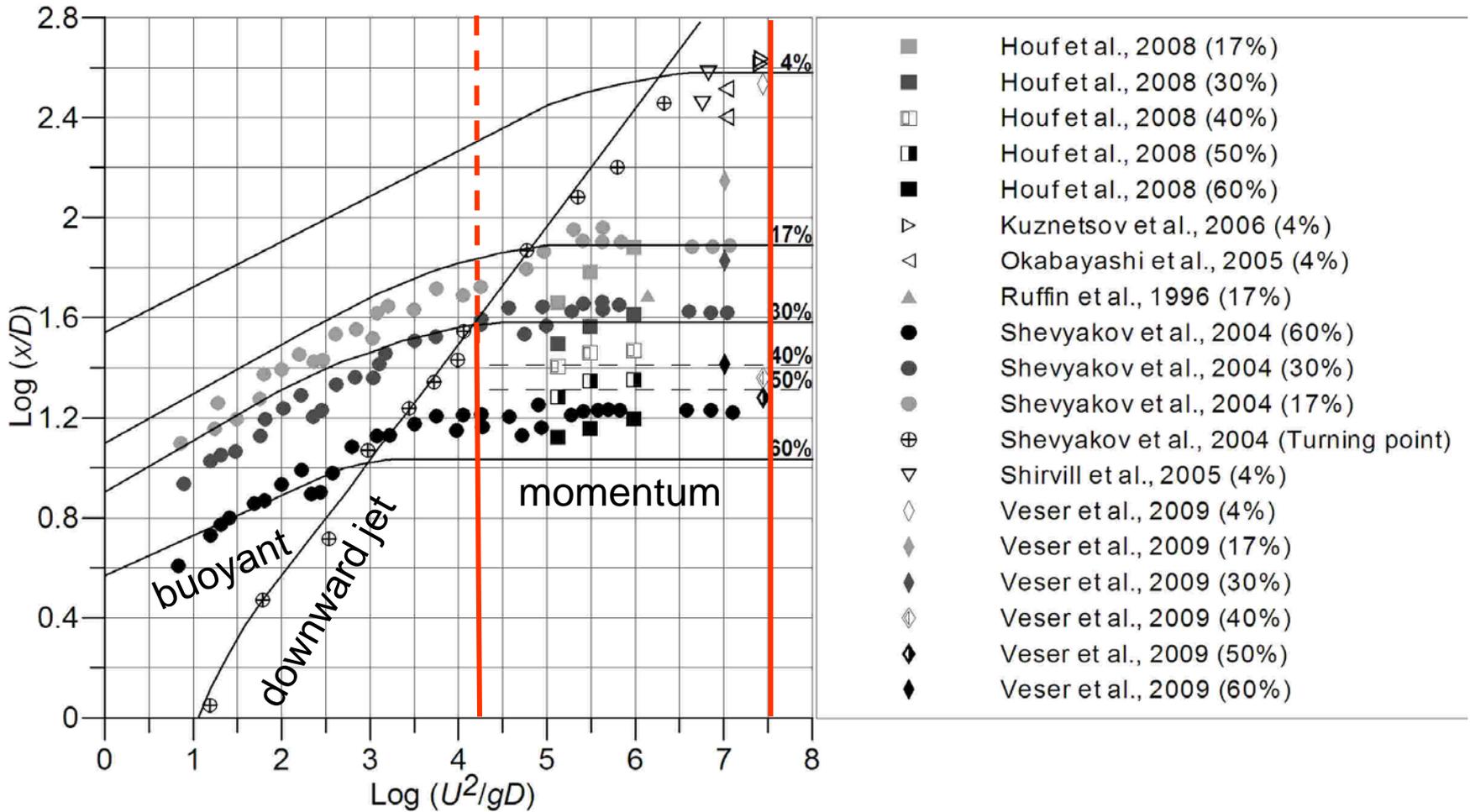
Buoyancy VS momentum jets

Buoyant jets decay faster than momentum jets (vertical)



When a jet becomes buoyant?

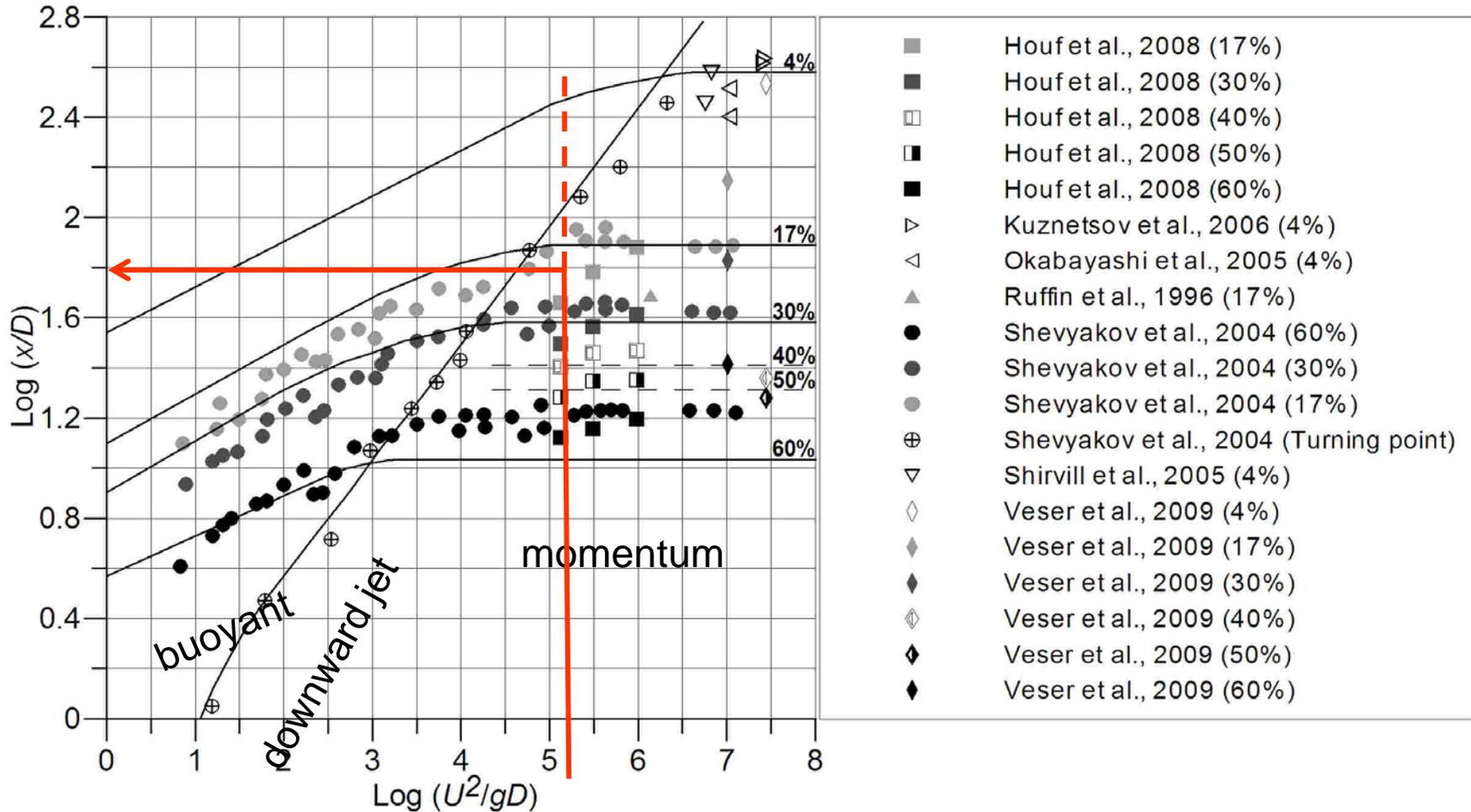
Start from the $Fr=U^2/gD$ (U and D real or notional nozzle)



Example: hydrogen pipeline (1/2)

- ❖ Since 1938 the chemical industries in Hüls, Ruhr area (Germany): 215 km, maximum pressure $P=25$ bar, inner diameter $D=16.8-27.3$ cm ($D_{\text{eff}}=98$ cm), full bore rupture mass flow rate $m=90$ kg/s: 15 cars/s (6 kg/fill), 3000 cars/3 min (time of fill), 1.4M cars/day, 10M cars/week (this pipeline would service 10M population), $\text{Log}(Fr=U^2/gD)=5.2$.
- ❖ If the similarity law is applied (assumption of momentum-controlled jet – conservative estimate) then horizontal distance to 4% by volume is ($\rho_N=1.267$) 465 m.
- ❖ If the Schevyakov's graph (previous slide) is applied in assumption of momentum-controlled jet at 4% then separation distance is ($\text{Log}(x/D)=2.63$) 418 m close to the similarity law result.

Example: hydrogen pipeline (2/2)



$$\text{Log}(U^2 / gD) = 5.2 \Rightarrow \text{Log}(x / D) = 2.04$$

Separation distance "reduction": **465 m to 107 m (4 times)**

Pressure effects of hydrogen unignited releases



Overlooked hydrogen safety issue

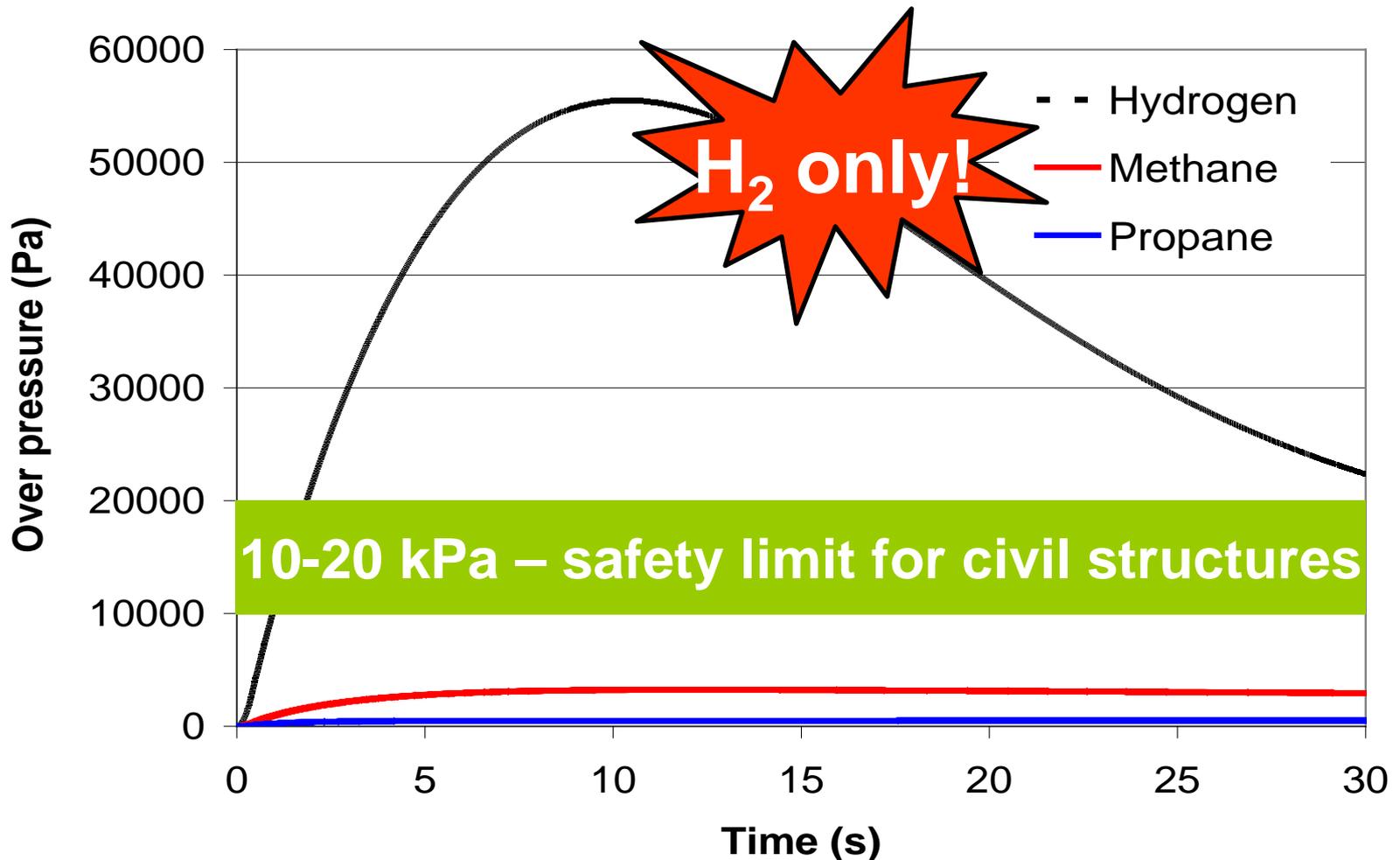
- **Example:** Hydrogen-powered car is in a closed garage of 44 m³ free volume. Release from an onboard storage through PRD of 5.08 mm diameter at pressure 350 bar gives mass flow rate 390 g/s (volumetric flow rate is $390/2 \times 0.02224 = 4.4 \text{ m}^3/\text{s}$).
- **Consequences:** Every second of non-reacting release pressure in the garage will increase by $(44+4.4)/44 = 1.1$ times, i.e. on 10 kPa. Civil building structures can withstand 10-20 kPa.
Thus, in 1-2 s the garage is “gone”.

Commercialisation of hydrogen in 2015...

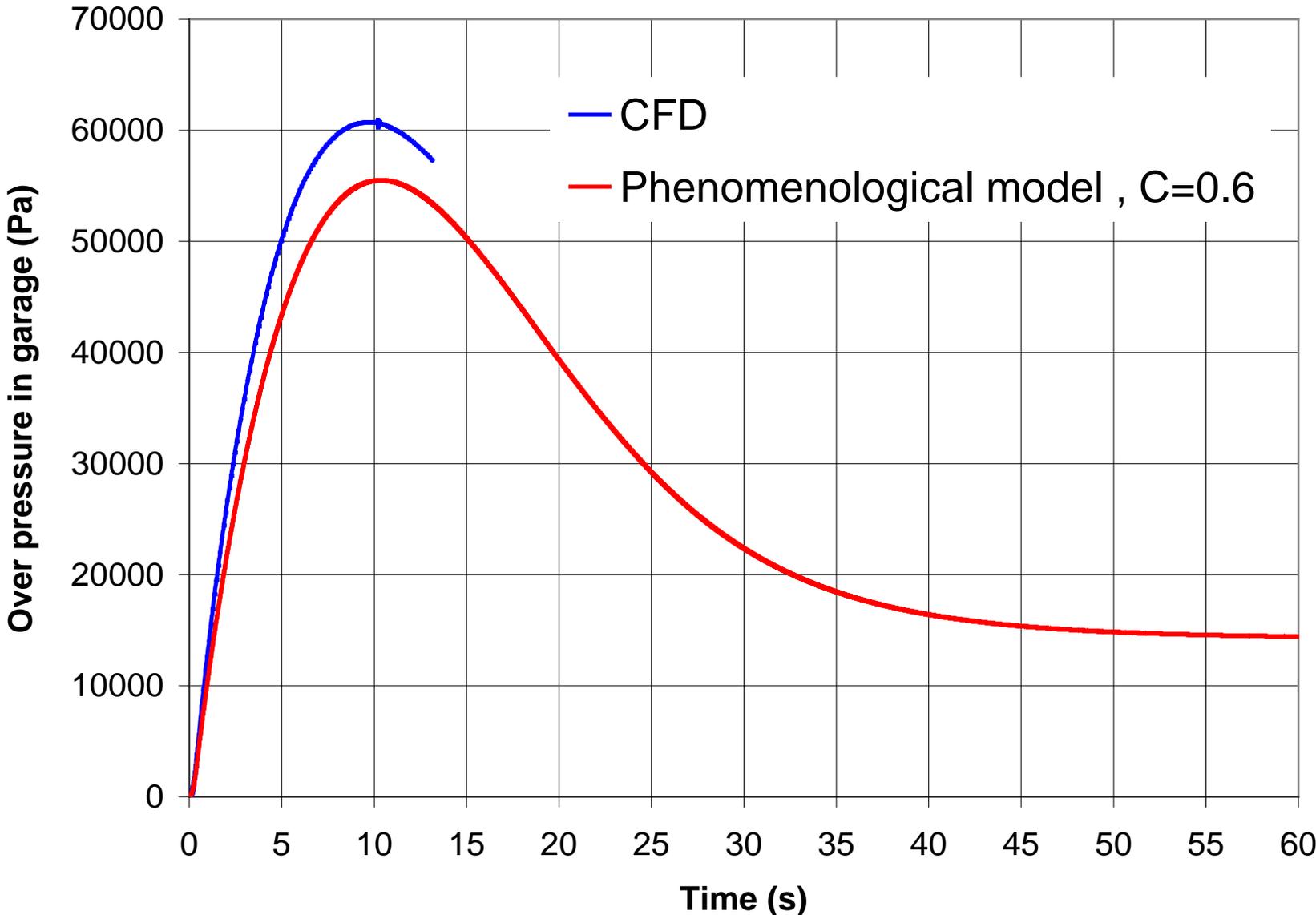
Pressure peaking phenomenon!

Small garage LxWxH=4.5x2.6x2.6 m (“brick” vent).

Mass flow rate 390 g/s (H₂: 350 bar, 5.08 mm orifice).

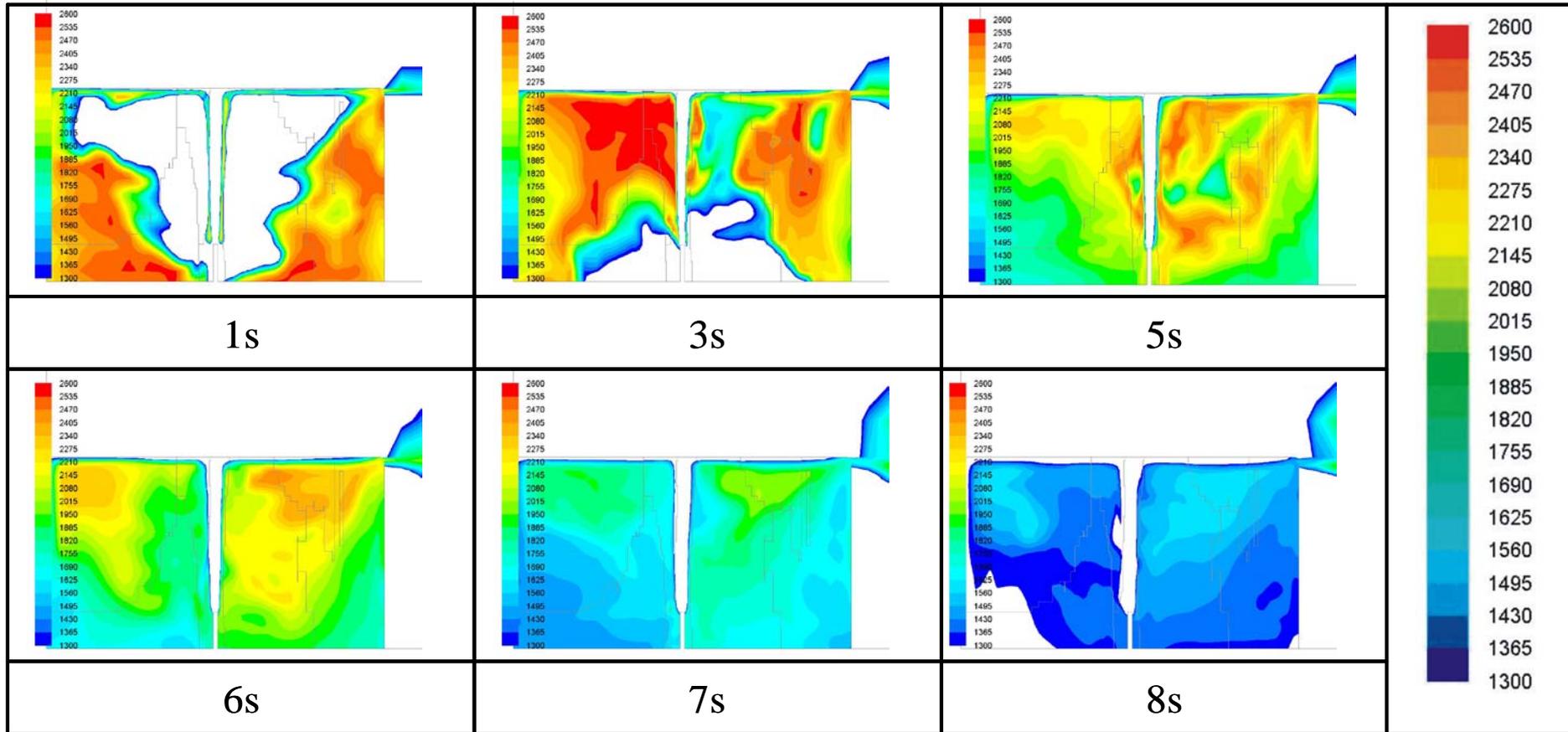


Pressure peaking: CFD vs simple model



Self-extinction of hydrogen fire

Current PRD with 390 g/s (350 bar, 5.08 mm)



Static temperature in the range 1300-2600 C



MSc in Hydrogen Safety Engineering (distance learning course):
<http://campusone.ulster.ac.uk/potential/postgraduate.php?ppid=24>