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MODELLING OF DISPERSION FOLLOWING HYDROGEN PERMEATION FOR SAFETY ENGINEERING AND RISK ASSESSMENT

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Introduction 1/3

- Viability of on-board hydrogen tanks depends on their gravimetric and volumetric capacity, leading to the use of high storage pressures and composite storage tank materials:
  - The pressure of hydrogen storage for automotive applications may be as high as 700 bar
  - Light-weight “Type IV” pressure vessels are likely to be used in automotive applications (polymer liner overwrapped by carbon fibre in resin matrix)
- Hydrogen permeability of the “Type IV” pressure vessels under high operating pressure is a safety concern

Introduction 2/3

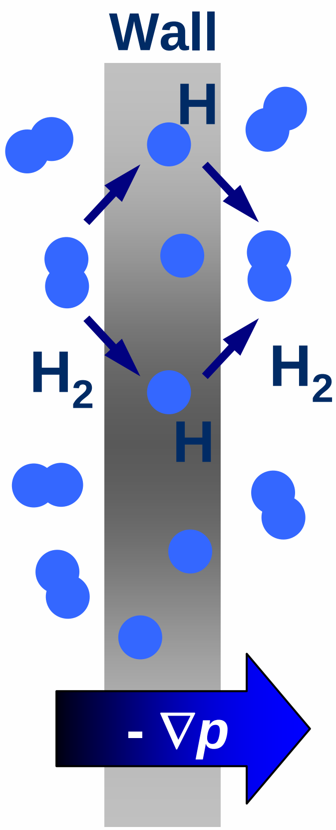
Permeation: “molecular diffusion through the walls or interstices of a container vessel, piping or interface material”

Ref.: SAE International, Technical information report J2579, January 2009, USA.

Permeability of materials, (mol H_2)·s^{-1}·m^{-1}·$MPa^{-1/2}$

Material	T=20⁰C	T=55⁰C
Fe (1)	5.47×10^{-11}	2.38×10^{-10}
High density polyethylene (2)	9.30×10^{-13}	3.17×10^{-12}
Carbon fibre/epoxy composite (2)	1.85×10^{-13}	5.79×10^{-13}
Stainless steel 303 (4)	4.09×10^{-16}	7.69×10^{-15}
Al (1)	2.47×10^{-24}	7.03×10^{-22}

(1) Yamanishi Y., Tanabe T., Imoto S. , 1983; (2) Humpenöder J. , 1998;
(3) Gorman J., Nardella W., 1962; (4) Korinko P., Scogin J., Clark E., 2001



Introduction 3/3

Proposals for H_2 permeability rate limit for vehicle RC&S:

Proposing standard	Max. allowable permeation rate	Units
Draft ISO15869:2004 (ambient temperature)	1.0	NmL/hr/L
ISO/TS 15869:2009 (Option i, Test B16, T=20^{0}C)	2.8@70MPa	NmL/hr/L
ISO/TS 15869:2009 (Option ii, Test E5, T=20^{0}C, end of the container life)	75	NmL/min per container
SAE J2579:01 2009 (min *T*=55^{0}C, end of the container life)	150	NmL/min per vehicle

Ref.: Adams P. et al., "Allowable hydrogen permeation rate from road vehicle compressed gaseous storage systems in garages: Part 1: Introduction, scenarios, and estimation of allowable permeation rate", in *Proc. 3rd Int. Conf. Hydrogen Safety*, 16-18 September 2009, Ajaccio, France.

Aim of research

Safety concern with hydrogen permeation: The formation of a flammable hydrogen-air mixture in closed space (e.g. a car in a garage with Type IV compressed hydrogen tank).

- Hydrogen concentration distribution in a garage with still air
- The interplay between hydrogen diffusion and buoyancy
- Hydrogen average concentration in an enclosure in assumptions of fully sealed garage and uniform hydrogen distribution

Problem formulation 1/2

- The assumed tank: L=0.672 m, ∅0.505 m, two hemispherical ends, 0.5m above ground (Area A_r=1.841 m^3, volume V_r=0.197 m^3)

http://world.honda.com/FCXClarity/package/index.html

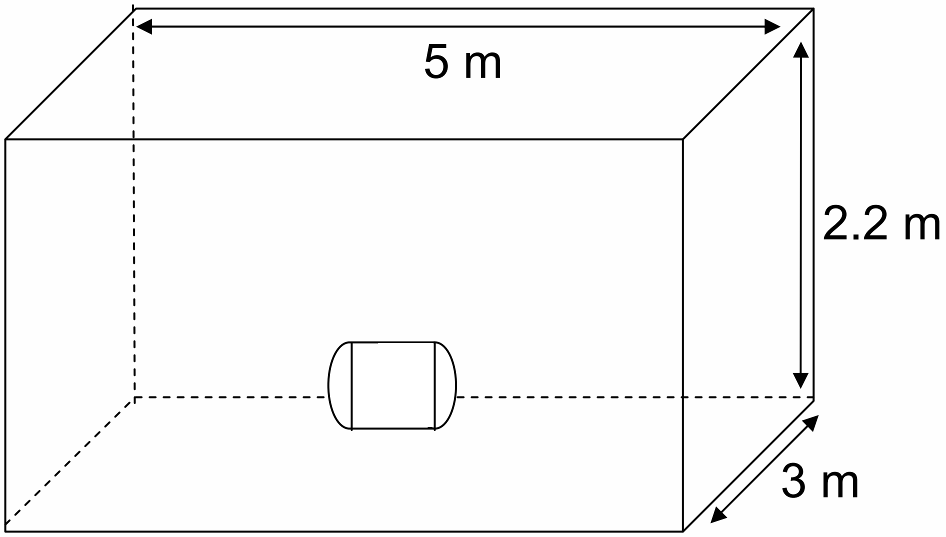
Sarkar A., Banerjee R. “Net energy analysis of hydrogen storage options”, *Int.J.Hydrogen Energy*, Vol. 30, pp.867–877 , 2005

- Permeation rates:
  – **$Q=6.25\times10^{-8}$ $m^3 \cdot s^{-1}$** (i.e. **1.14 $NmL \cdot hr^{-1} \cdot L^{-1}$**, close to Draft ISO15869:2004)
  – **$Q=1.92\times10^{-6}$ $m^3 \cdot s^{-1}$** (i.e. **35.0 $NmL \cdot hr^{-1} \cdot L^{-1}$**, close to ISO/TS 15869:2009 & SAE J2579:01 2009)

Problem formulation 2/2

- The typical garage: *L*=5 m, *W*=3 m, *H*=2.2 m
- Assumed perfectly sealed

Ref.: Sarkar A., Banerjee R. “Net energy analysis of hydrogen storage options”, *Int.J.Hydrogen Energy*, Vol. 30, pp.867–877 , 2005.



CFD model of H_2 permeation

- 3D unsteady Navier-Stokes equation set, laminar flow
- SIMPLE algorithm
- 3rd order MUSCL discretisation scheme for convective terms, central difference for diffusion terms
- 4-stage Runge-Kutta time stepping scheme
- H_2 release:

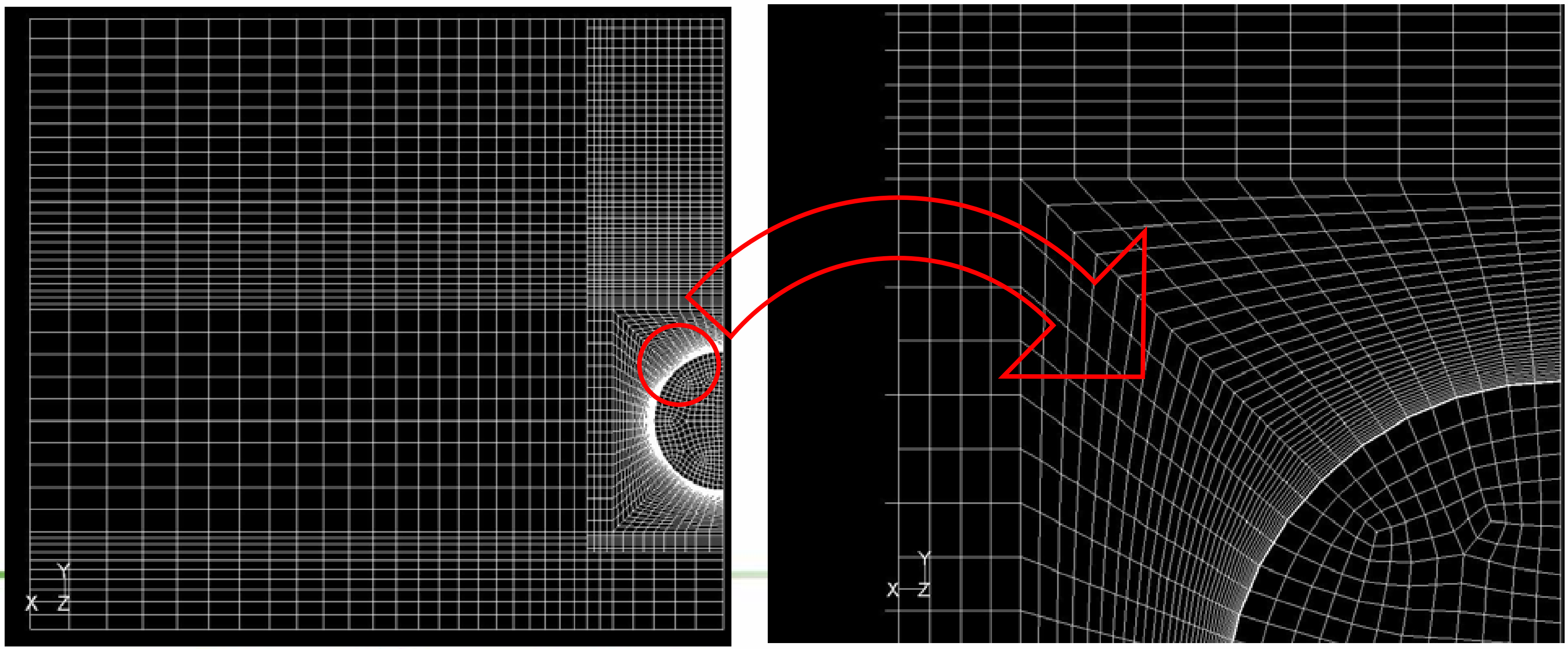
  volumetric source (2 CVs, 1.0 mm total thickness)

  1.14 $NmL \cdot hr^{-1} \cdot L^{-1} \Rightarrow S_{H2}=2.61\times10^{-6}\ kg \cdot s^{-1} \cdot m^{-3}$

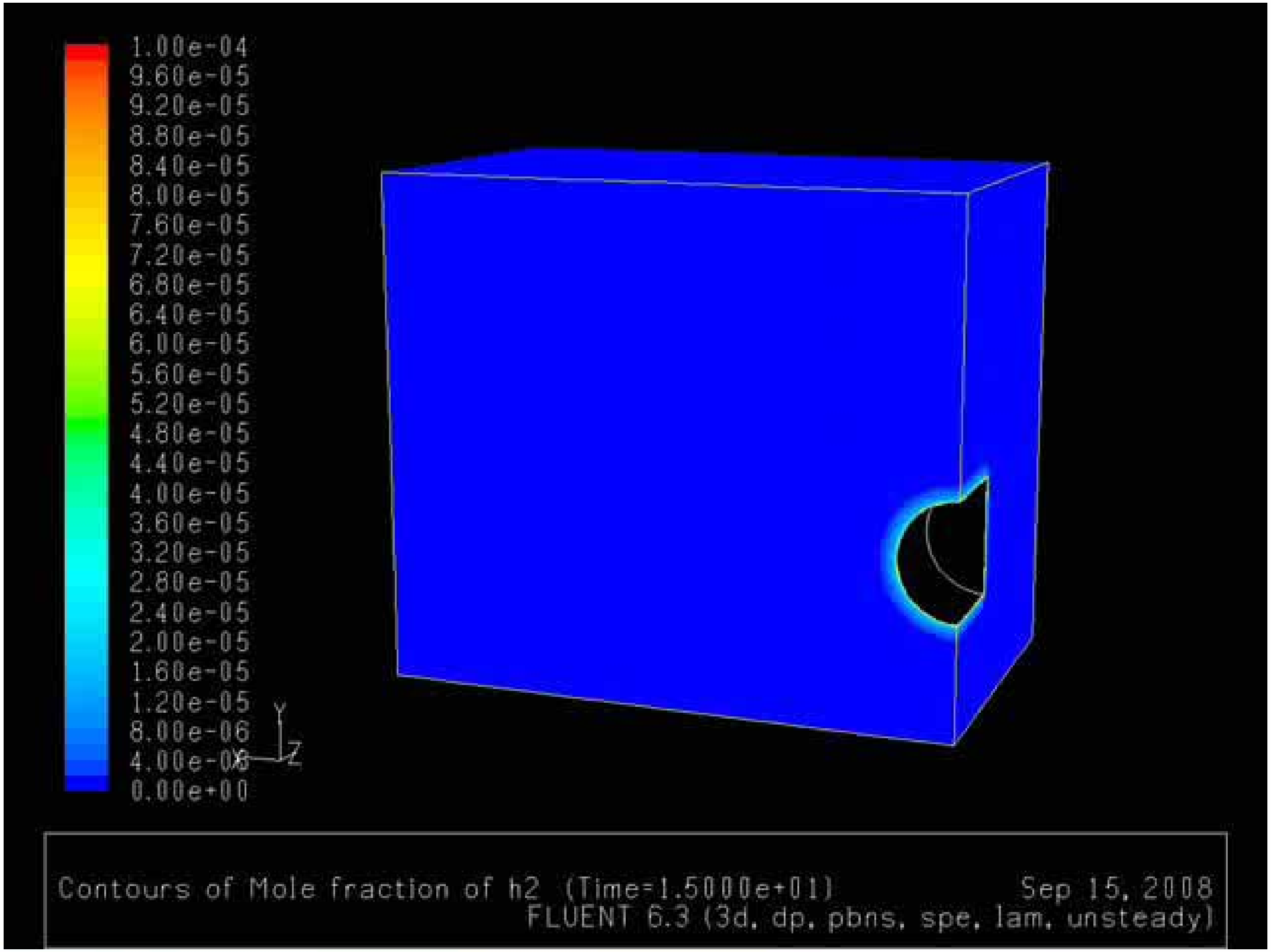
  35.0 $NmL \cdot hr^{-1} \cdot L^{-1} \Rightarrow S_{H2}=8.53\times10^{-5}\ kg \cdot s^{-1} \cdot m^{-3}$
- Time step: Δt=0.05 s (max V=0.0215m/s, CFL_{MAX}=0.06, cell Re_{MAX}~100)

Calculation domain and grid

- ¼ of the garage (dissected along symmetry planes)
- LxDxH=2.5x1.5x2.2m
- Δ_{CV}=0.5mm (next to the cylinder surface), 194,464 control volumes altogether
- H_2 release volume: 1mm thick envelope, $V=4.6 \cdot 10^{-6}\ m^3$
- Outflow vent: 0.1x0.1m, positioned at the floor centre

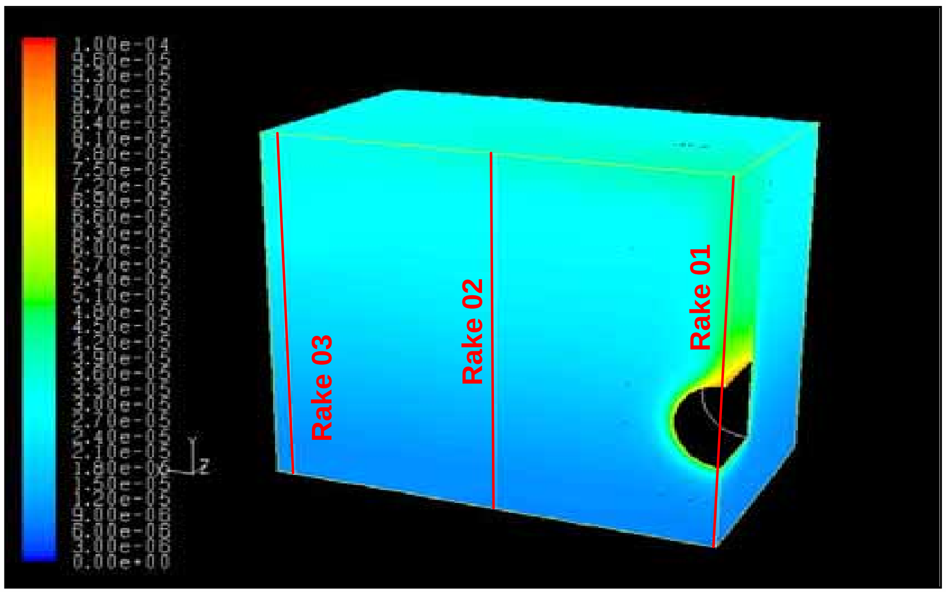


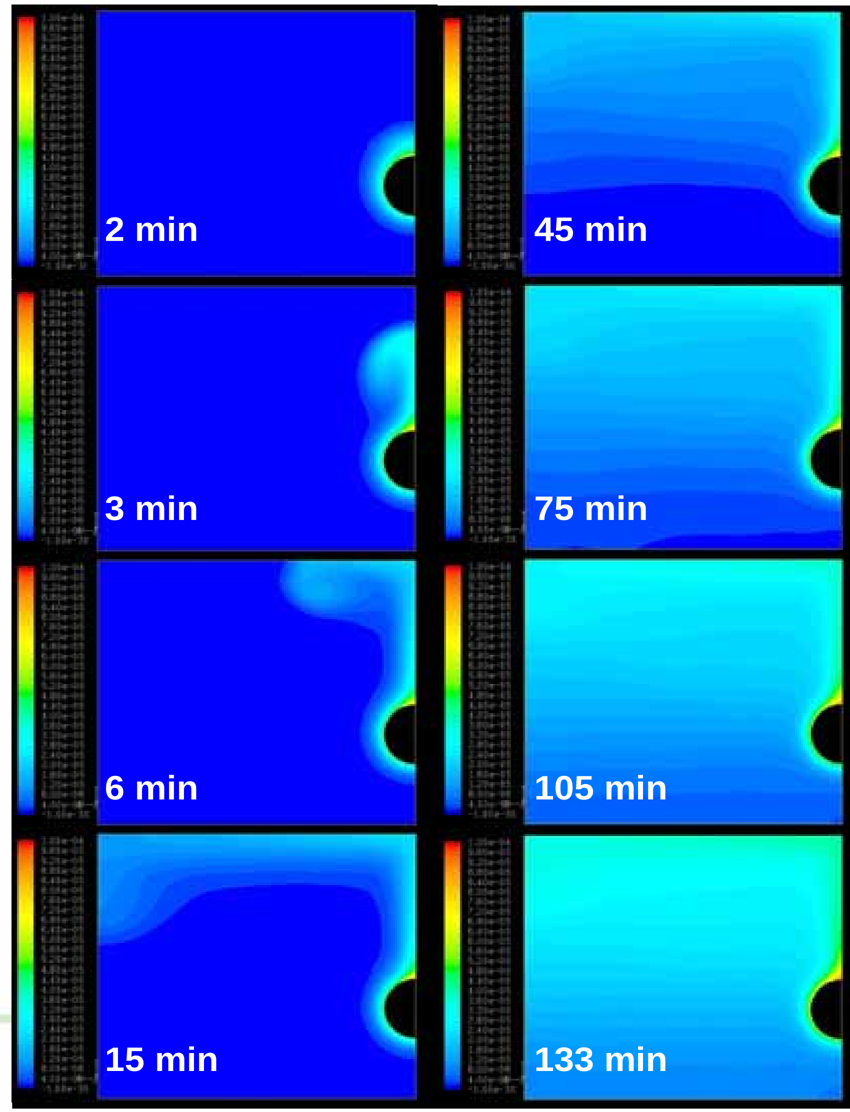
Simulation results (1.14 $NmL \cdot hr^{-1} \cdot L^{-1}$)



Simulation results (1.14 NmL·hr^{-1}·L^{-1})

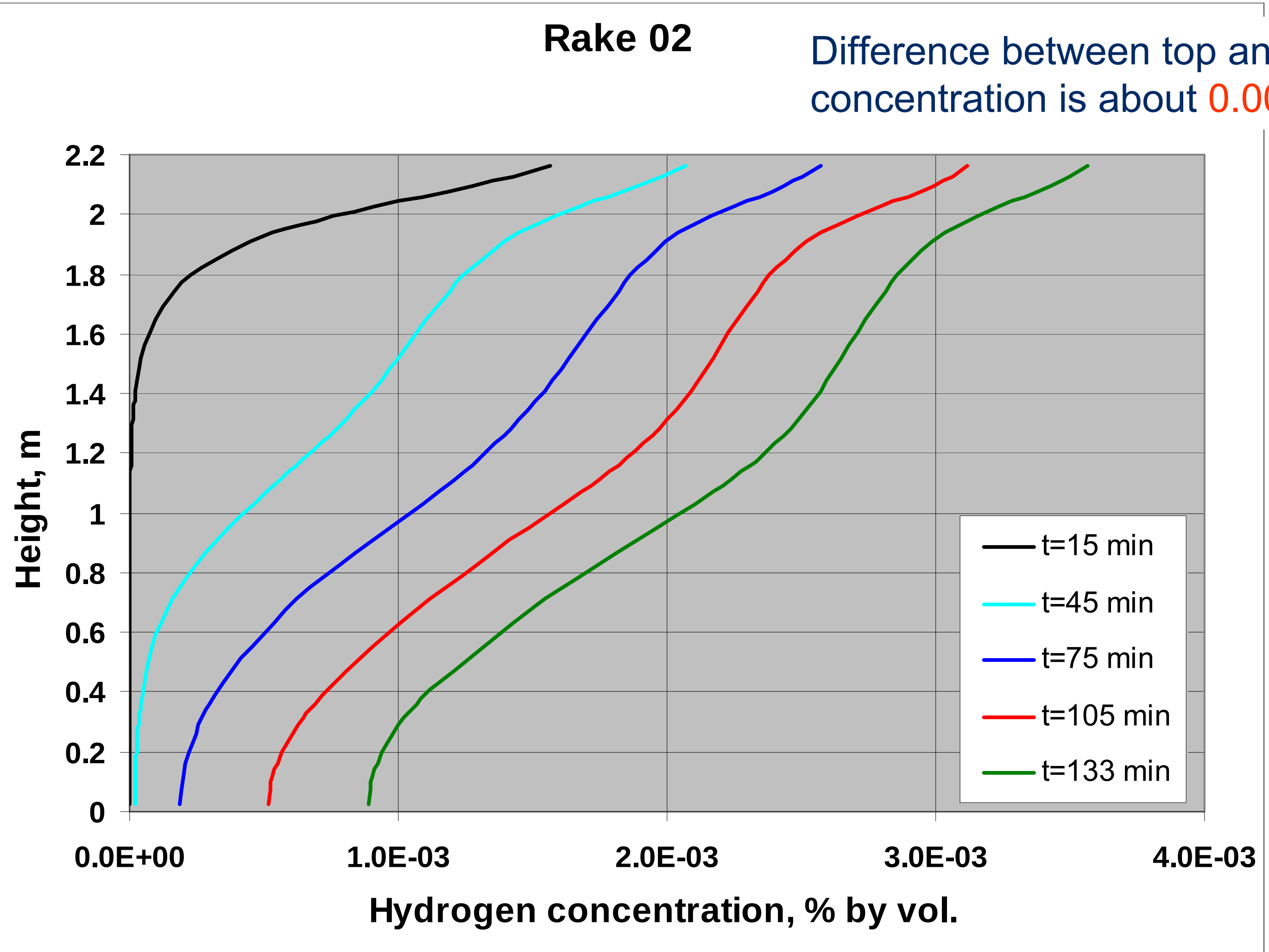
Hydrogen concentration distribution along three rakes



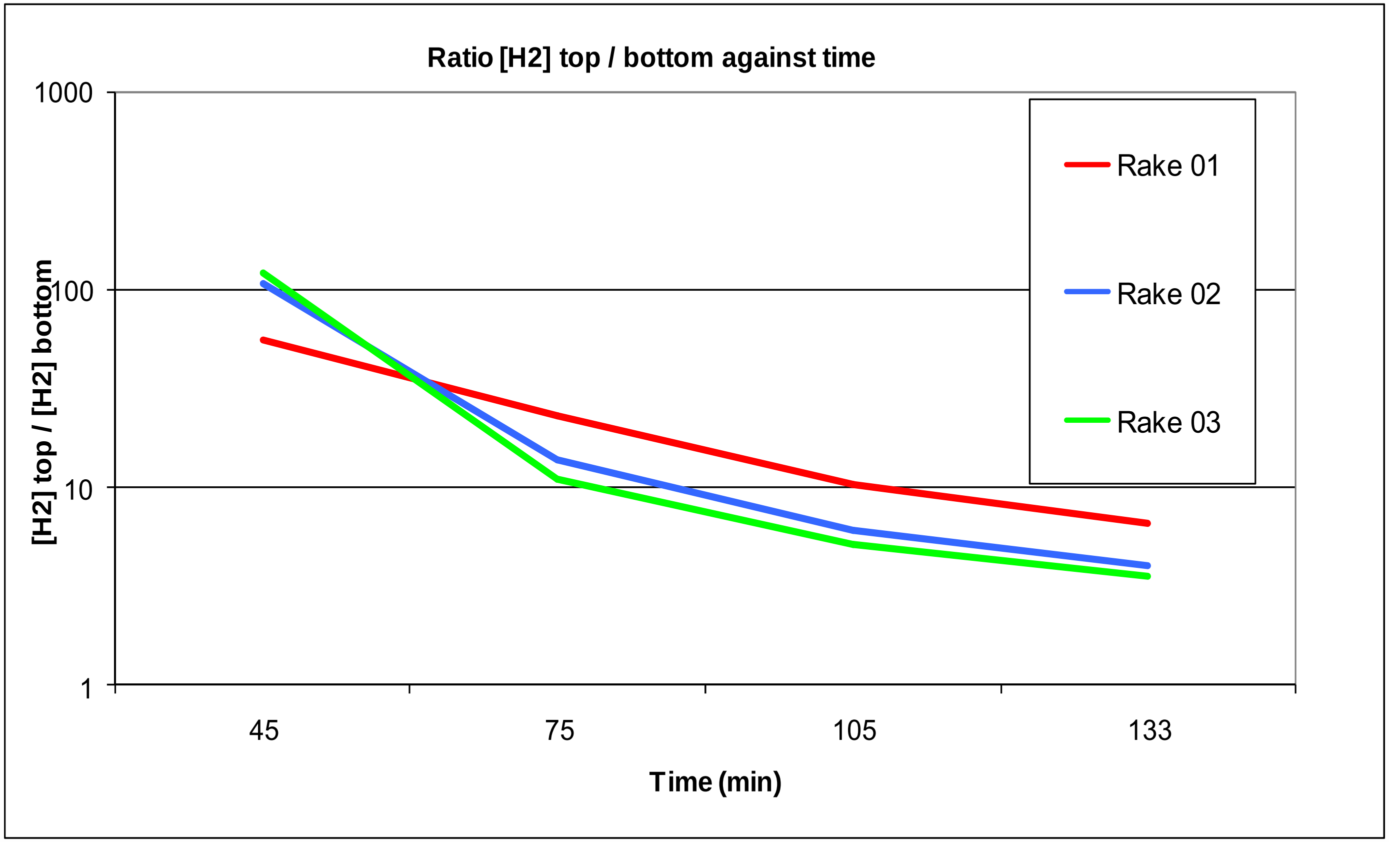


Simulation results (1.14 $NmL \cdot hr^{-1} \cdot L^{-1}$)

Difference between top and bottom H_2 concentration is about 0.002% vol.



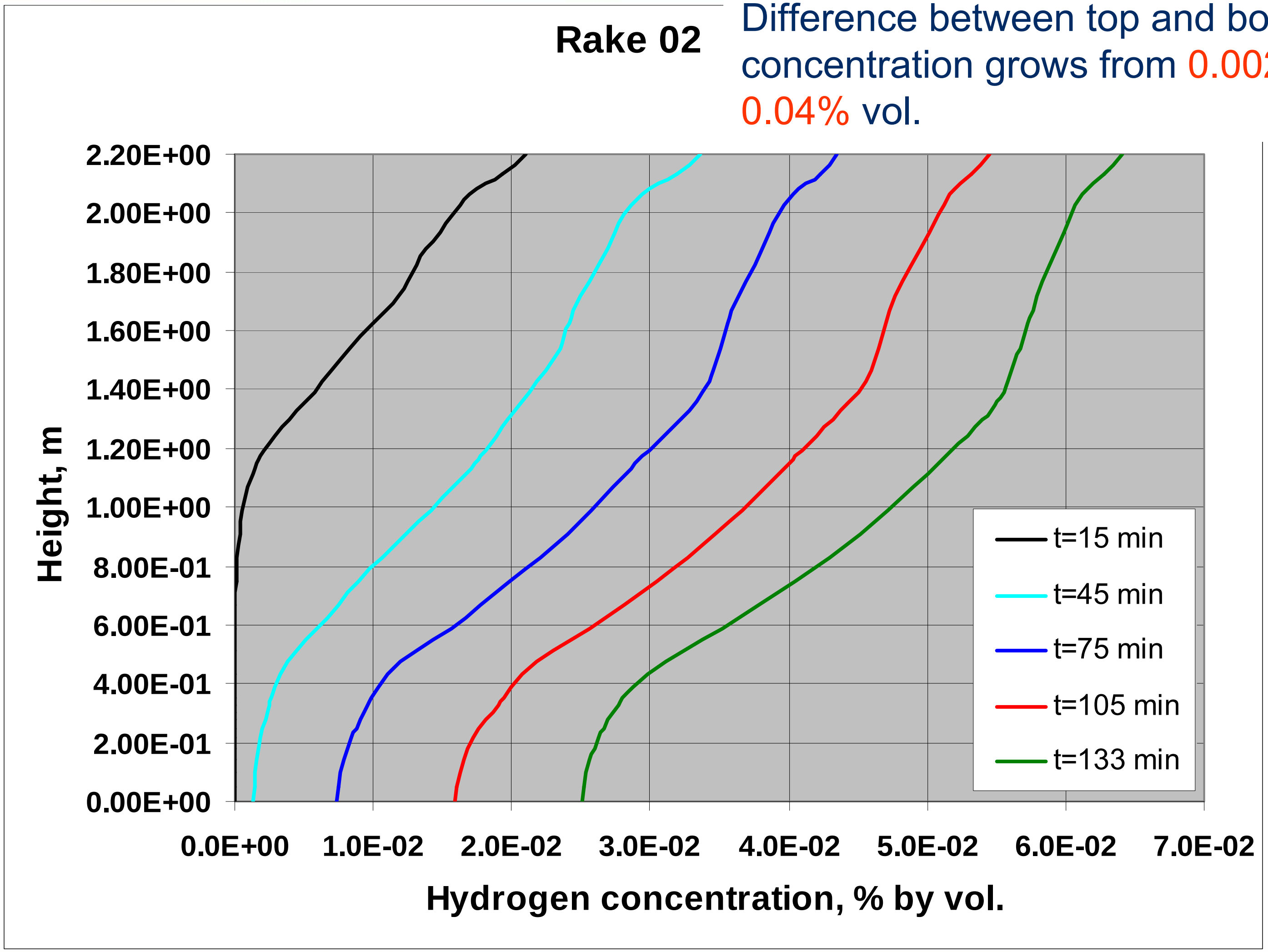
Simulation results (1.14 $NmL \cdot hr^{-1} \cdot L^{-1}$)



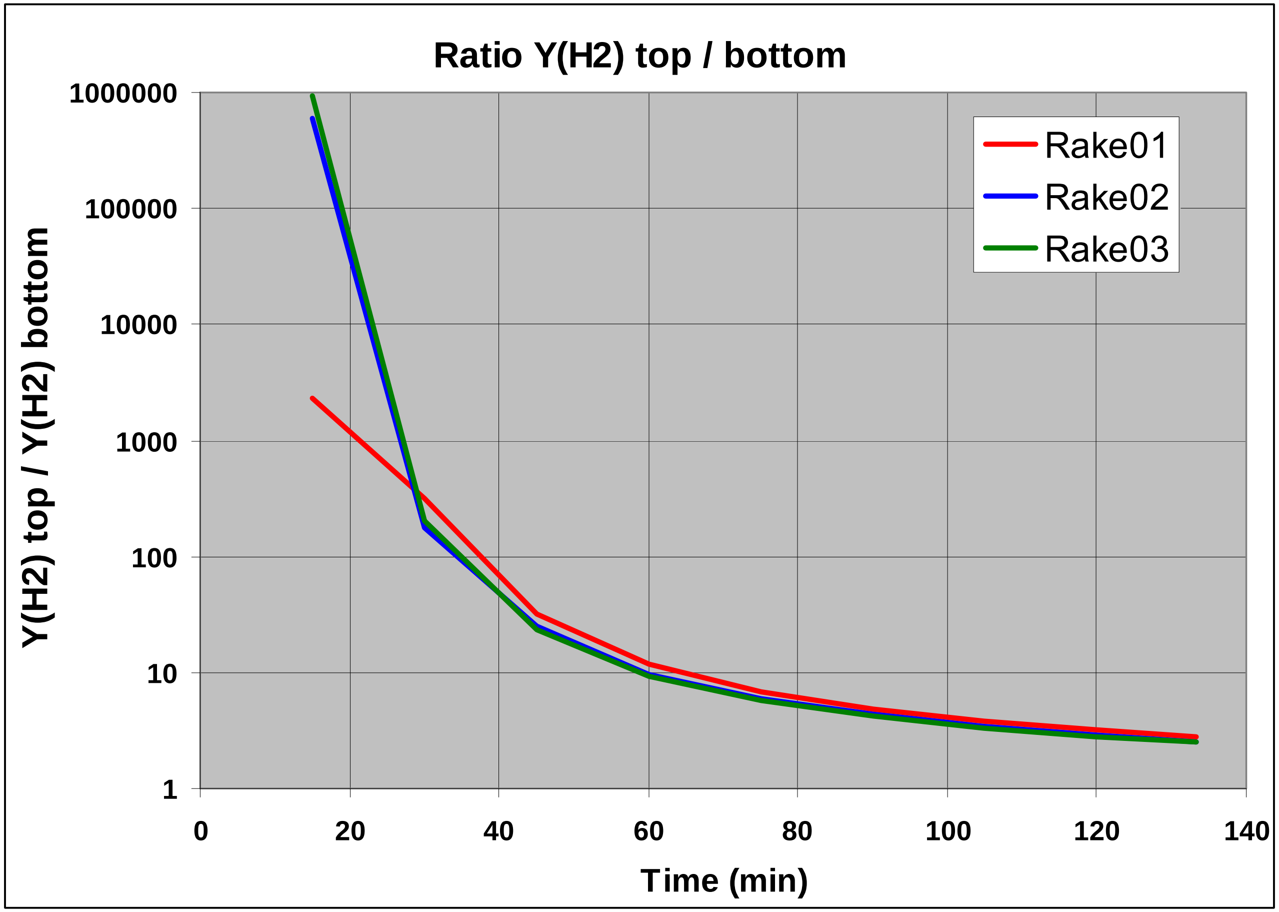
Hydrogen-air mixture across the garage tends to be homogenous with time!

Simulation results (35 $NmL \cdot hr^{-1} \cdot L^{-1}$)

Difference between top and bottom H_2 concentration grows from 0.002% vol. to 0.04% vol.



Simulation results (35 NmL·hr^{-1}·L^{-1})



Hydrogen-air mixture across the garage tends to be homogenous with time!

Conclusion

- The used rate of permeation in our scenarios does not represent a safety issue:
  - Low concentration on surface and in garage, and quasi-uniform distribution,
  - In a perfectly closed garage H_2 concentration reaches 4% vol. after ~240 days for 1.14 $NmL \cdot hr^{-1} \cdot L^{-1}$ permeation rate and ~ 8 days for 35 $NmL \cdot hr^{-1} \cdot L^{-1}$,
  - Over-conservative assumptions (perfectly sealed garage, still air, no temperature gradient).
- Both ISO/TS 15869:2009 and SAE J2579:01 2009 regulations tend to be conservative.

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Thank you for your attention!

Acknowledgement:

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