Numerical modeling of a moderate hydrogen leak in a 1m^3 enclosure with two vents

E Saikali, P Ledac, A Bruneton, A Khizar, C Bourcier, G Bernard-Michel, E Adam

Université Paris-Saclay, CEA - DES/ISAS/DM2S/STMF/LGLS, Gif-sur-Yvette, France

D Houssin-Agbomson

Air Liquide R& D - Innovation Campus Paris, Les loges-en-Josas, France

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Hydrogen (H_2) energy applications

- **Application domains**

Transport (fuel cells, forklifts, cars, emergency backup systems),

Energy conversion,

Hydrogen usage (city gas, combustion).

- **Advantages**

Green vector of energy (no CO_2),

High energy capacity storage.

- **Disadvantages**

H_2/air mixture is highly flammable,

Transparent flame.

- **Requirements: R & D**

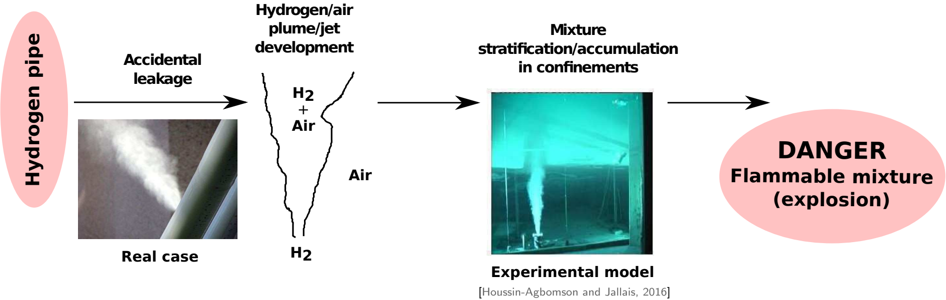
Security, production, storage and distribution (costs, capacity).

Left: [Houssin-Agbomson and Jallais, 2016], right: personal document (ICHS2017, Hambourg).

- **Most frequent accidental scenario**

Moderate H_2 leakage in confined environments (technical/human error),

Concentration stratification/accumulation.



Schematic description of the most frequent H_2 leakage accidental scenario.

- **Risk mitigation**

Passive ventilation: reduce H_2 accumulation from leakage scenarios.

- **Simplified models**

Idealized fuel cell models: H_2 release in confined/semi-confined environments.

DRHyS experimental cavity (CEA - Air liquide)

- **In the present work we model**

Moderate H2 leak (10.4 Nl.min^{-1}) in a two vented configuration (1 m^3),

Injection pipe of diameter $d = 2.72$ cm, release point centered at height 8 cm,

Two vents 96 x 18 cm^2 (opposite walls, bottom and top) ,

Assume that the iso-thermal/bar conditions are valid ($T = 11^\circ$ C, $P_{\text{thm}} = 1$ bar),

[Bernard-Michel and Houssin-Agbomson, 2017]

Available experimental data: H2 concentration at 15 minicatharometers

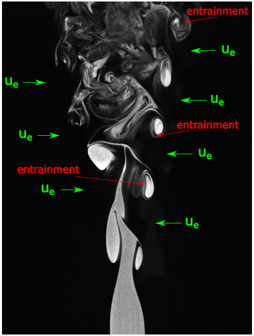
Industrial theoretical approach (desired)

- **Easy, fast ... but some limitations**
- **Linden's based on MTT** [Morton et al., 1956]

Three assumptions:

- Entrainment ($u_e = \alpha \mathcal{W}$),
- Boussinesq approximation,
- Self-similar solutions.

α entrainment coefficient (assumed constant),
u_e entrainment horizontal velocity,
$\mathcal{W}$ characteristic vertical velocity.



CEA private communication

- **Entrainment assumption experimental validations in free media**

Better predictions reported with $\alpha(z, \mathrm{Ri})$ [Abraham, 1965], [List and Imberger, 1973].

- **Further induced difficulties**

Non-Boussinesq flows,

Confined/semi-confined media.

Alternative approach: CFD !!

CFD: advantages, issues & challenges

- **Advantages**

Access all flow variables + 3D description (velocity, concentration, pressure, . . .)

- **Physical issues**

Air & H2: $\rho_{\text{amb}}/\rho_{\text{inj}} \approx 14$,

Non-stationary fluctuating regime,

Laminar-turbulent transition,

Interior/exterior interactions.

- **Numerical issues**

Low Mach Number vs Boussinesq
[Gray and Giorgini, 1976],

Turbulence models and schemes:
(transition and sharp gradients),

Open boundary conditions
[Desrayaud et al., 2013].

- **Challenges**

Modeling . . .

Turbulent scales: inertia & mixing (can be very small),

Robust CFD & HPC software,

Cost, resources, . . .

- **Benchmark: CFD vs exp** (1 m^3)

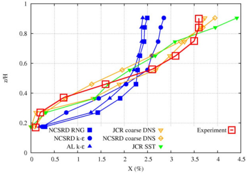
[Bernard-Michel et al., 2013], [Tran et al., 2013]

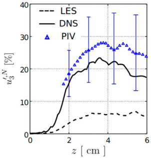
Maximum He concentration (3.5%)

- overestimated in axi-symetric calculations,
- overestimated without turbulence model (coarse mesh),
- underestimated with FANS (Favre).

Homogeneous layer

- predicted only with FANS.





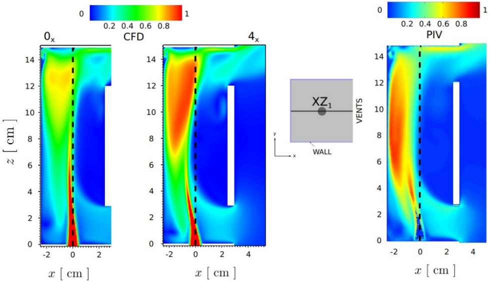
- **Mini-GAMELAN** (3.7x10^{-4} m^3)

[Saikali et al., 2019], [Saikali et al., 2020]

LES vs DNS

- underestimated fluctuations,
- plume structure,

BC treatment: should be modeled!



- **Numerical modeling**

DNS: no turbulence modeling (solve all scales),

Model injection and outer regions,

Simulate a steady-state solution.

Main objectives

- Reproduce the bi-layer concentration regime (Linden + exp data),

- Provide a complete flow pattern description (cross-flow, distribution, ...),

- Provide 3D reference data that can serve for improving industrial models (α).

- **CFD software HPC**

TRUST open source code: **https://github.com/cea-trust-platform/trust-code**

Conservation equations (mass, momentum, species) + equation of state,

LMN asymptotic analysis $\rightarrow P_{\text{tot}}(\mathbf{x}, t) = \underbrace{p(t)}_{\text{thermodynamic}} + \widetilde{\text{Ma}}^2 \underbrace{P(\mathbf{x}, t)}_{\text{hydrodynamic}}$.

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial}{\partial x_i}(\rho u_i) = 0, \\ \dfrac{\partial \rho u_j}{\partial t} + \dfrac{\partial}{\partial x_i}(\rho u_j u_i) = -\dfrac{\partial P}{\partial x_j} + \dfrac{\partial \tau_{ij}}{\partial x_i} + \rho g_j, \\ \dfrac{\partial \rho Y_1}{\partial t} + \dfrac{\partial}{\partial x_i}(\rho Y_1 u_i) = \dfrac{\partial}{\partial x_i}\left(D\rho \dfrac{\partial Y_1}{\partial x_i}\right), \\ \rho = \dfrac{p}{RT}\left(\dfrac{Y_1}{M_{\text{inj}}} + \dfrac{Y_2}{M_{\text{amb}}}\right)^{-1}. \end{cases}$$

ρ mixture's density, Y mass fraction, M molar mass,

$\tau_{ij} = 2\mu e_{ij}, e_{ij} = S_{ij} - \frac{1}{3}\delta_{ij}S_{kk}, S_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right), Y_2 = 1 - Y_1,$

$\mathbf{u} = (u_i)$ velocity field, $\mu(\mathbf{x}, t)$ mixture's dynamic viscosity,

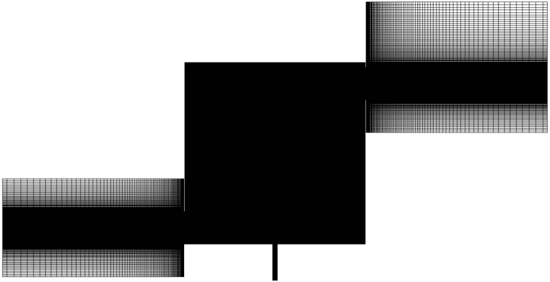
$D = 7.72 \times 10^{-5}$ m^2.s^{-1} is the diffusion coefficient (uniform & constant).

- **Meshing**

Open source SALOME platform

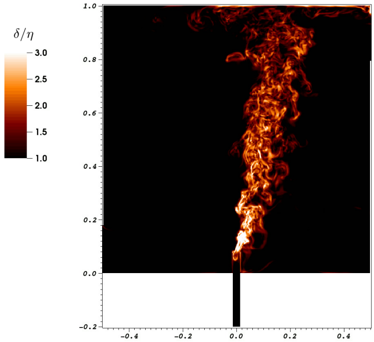
Two hexahedral non-uniform unstructured meshes

- 250 million & 2 billion cells,
- $\delta \approx 1$ mm - 4 cm & 0.5 mm - 2 cm
- 5K & 50K MPI procs respectively.



https://www.salome-platform.org/

- **Kolmogorov scale**



- **Cost**

Physical time

- 3.5 min (mesh 1)
- 0.5 min (mesh 2 - resumed)

Resources

$\approx$ 12 M hours, IRENE-ROME

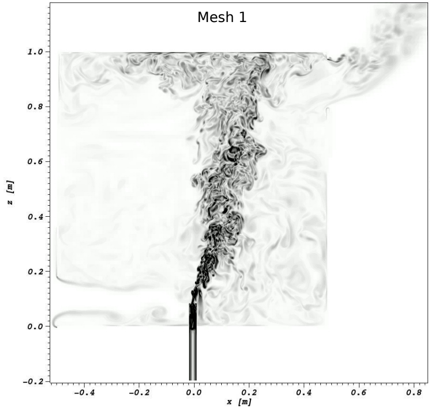
Interpolation & initial conditions

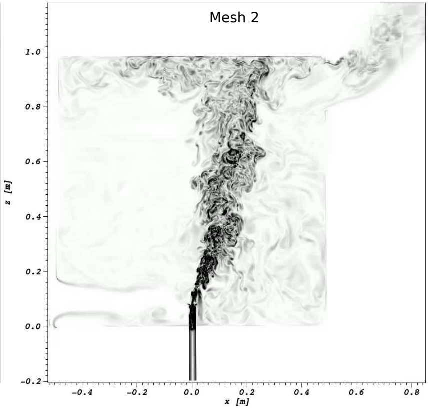
- **Mesh 1**

Simulated until reaching a steady state (≈ 1 min of physical time),

- **Mesh 2**

Parallel interpolator of MEDCoupling for initializing the fine simulation.



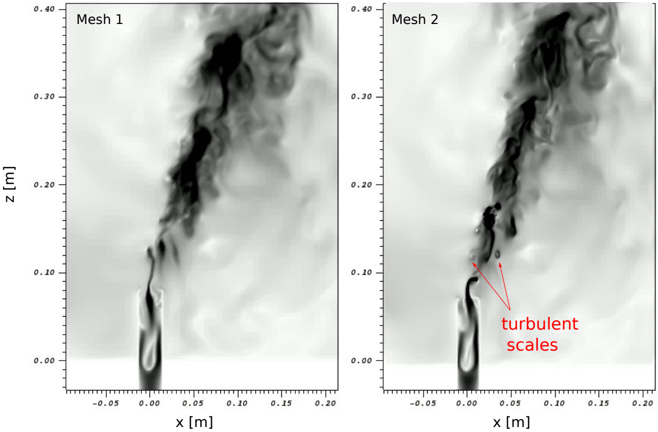


Fine resolution

- **Comparisons**

Same deviation which means same cross-flow effect,

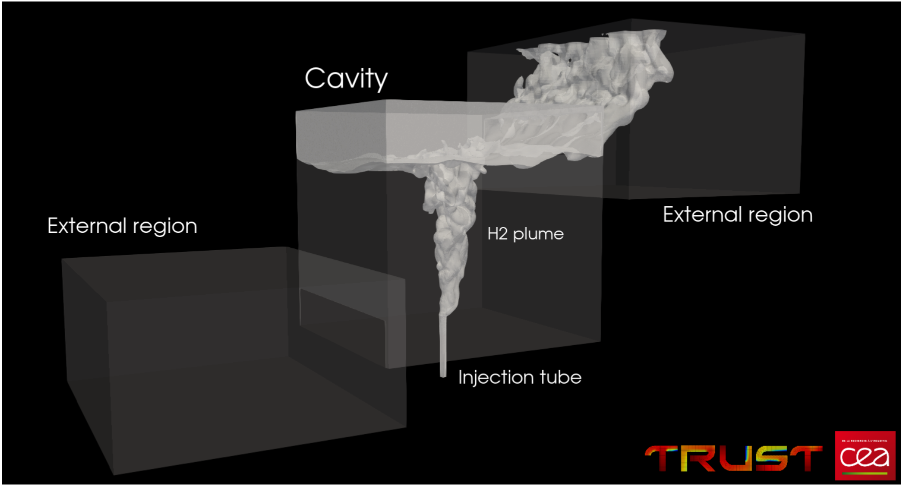
Mesh 2 captures **(better)** the small structures (mainly at the jet border),



- **H2 iso-volumes** (1.5 %)

Upper interface, deviation + deformation, turbulent (qualitative),

Cavity sufficiently large to avoid plume/wall interactions (Coanda effect).

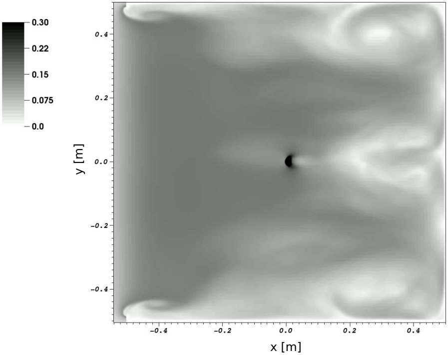


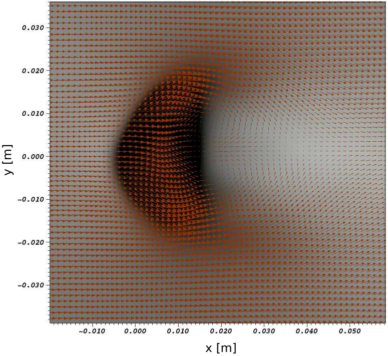
- **Velocity magnitude time-averaged iso-contours**

Horizontal 2D slice ($z = 0.1$ m),

Symmetrical distribution, counter-rotating vortices, jet deviation/deformation,

Behavior reproduced previously in [Saikali et al., 2019], [Saikali et al., 2020]





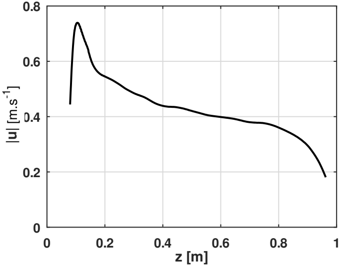
- **Axis deviation**

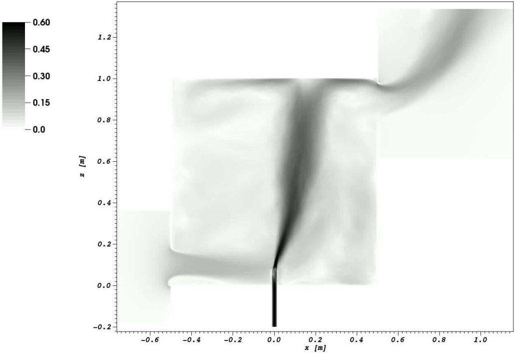
Heavy air pushes light H2 to the right,

Entrainement + gravity accelerations keep an upward direction afterwards,

- **Axial evolution**

Transition + plume regions
[Saikali et al., 2020]





- **Inflow**

Almost uniform,

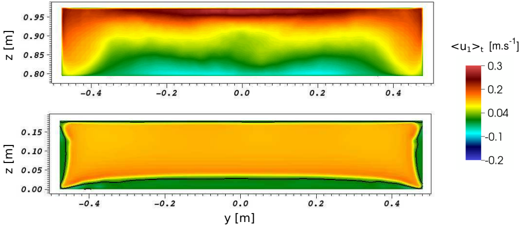
Classical profile (inverted parabola).

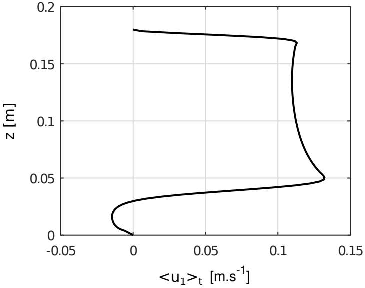
- **Outflow**

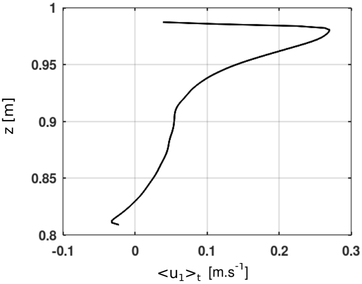
Thin exiting jet,

Back-flow in a shear-layer,

More statistical recording in progress.







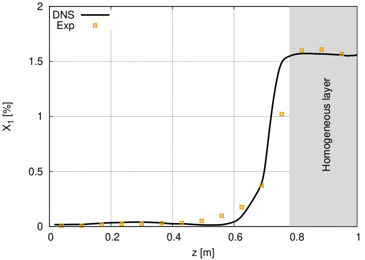
- **H2 iso-contours [0-5%]**

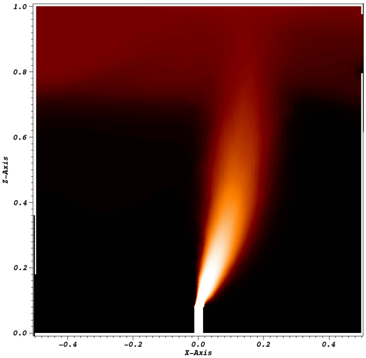
A clear bi-layer distribution,

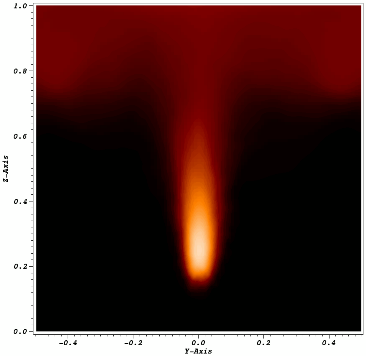
System well ventilated (for this configuration),

Very good agreement with experiment,

Maximal concentration far from risk range ...







DNS results presented for a moderate H2 leakage in a 1 m^3 vented cavity,

Results are in good agreement with experimental measurements,

Results show that CFD is a good approach . . . if well resolved,

The ventilation system is very good (for the treated configuration),

Important cross-flow effect . . . but the cavity is large !

The recorded concentration regime is far from the risk range.

- **Prospects**

Employ the reference 3D data to model α (continuation of [Saikali et al., 2020]),

Improve the boundary conditions (profiles to impose on the vent surface directly).

Thanks for your attention!!

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https://github.com/cea-trust-platform/trust-code

Velocity magnitude iso-contours in the mid-vertical plane

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Abraham, G. (1965).
Entrainment principle and its restrictions to solve problems of jets.
Journal of Hydraulic Research, 3(2):1–23.

Bernard-Michel, G., Cariteau, B., Ni, J., Jallais, S., Vyazmina, E., Melideo, D., Baraldi, D., and Venetsanos, A. (2013).
Cfd benchmark based on experiments of helium dispersion in a 1 m3 enclosure–intercomparisons for plumes.
In *Proceedings of ICHS 2013*.

Bernard-Michel, G. and Houssin-Agbomson, D. (2017).
Comparison of helium and hydrogen releases in 1 m 3 and 2 m 3 two vents enclosures: Concentration measurements at different flow rates and for two diameters of injection nozzle.
International Journal of Hydrogen Energy, 42(11):7542–7550.

Desrayaud, G., Chénier, E., Joulin, A., Bastide, A., Brangeon, B., Caltagirone, J., Cherif, Y., Eymard, R., Garnier, C., Giroux-Julien, S., et al. (2013).
Benchmark solutions for natural convection flows in vertical channels submitted to different open boundary conditions.
International Journal of Thermal Sciences, 72:18–33.

Gray, D. D. and Giorgini, A. (1976).
The validity of the boussinesq approximation for liquids and gases.
International Journal of Heat and Mass Transfer, 19(5):545 – 551.

Houssin-Agbomson, D. and Jallais, S. (2016).
Développement d'outils d'ingénieurs pour l'évaluation du risque hydrogène.
6A-Risques liés aux nouveaux usages-architectures robustes 2.

List, E. J. and Imberger, J. (1973).
Turbulent entrainment in buoyant jets and plumes.
Journal of the Hydraulics Division, 99(9):1461–1474.

Morton, B. R., Taylor, G. I., and Turner, J. S. (1956).
Turbulent gravitational convection from maintained and instantaneous sources.
Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, 234(1196).

Bibliography II

Saikali, E., Bernard-Michel, G., Sergent, A., Tenaud, C., and Salem, R. (2019).
Highly resolved large eddy simulations of a binary mixture flow in a cavity with two vents: Influence of the computational domain.
International Journal of Hydrogen Energy, 44(17):8856–8873.

Saikali, E., Sergent, A., Wang, Y., Quere, P. L., Bernard-Michel, G., and Tenaud, C. (2020).
A well-resolved numerical study of a turbulent buoyant helium jet in a highly-confined two-vented enclosure.
International Journal of Heat and Mass Transfer, 163:120470.

Tran, H. L., Sergent, A., Bernard-Michel, G., and Le Quere, P. (2013).
Numerical simulation of the helium dispersion in a semi-confined air-filled cavity.
In *Progress in safety of hydrogen technologies and infrastructure: enabling the transition to zero carbon energy. Proceedings of the 5th International Conference on Hydrogen Safety (ICHS). 9-11 Sept 2013, Brussels, Belgium*.