Numerical simulation of Helium dispersion in a semi-confined air-filled cavity

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2. Configuration
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4. Numerical methods and validation
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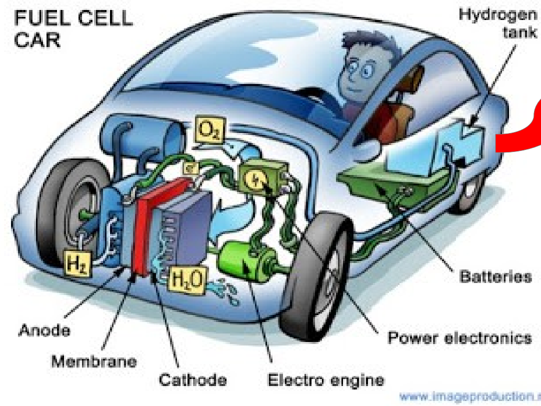
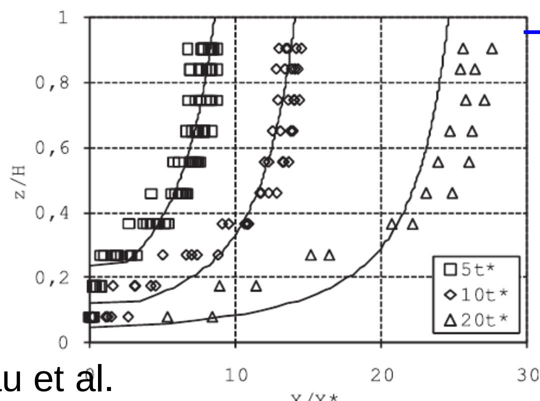
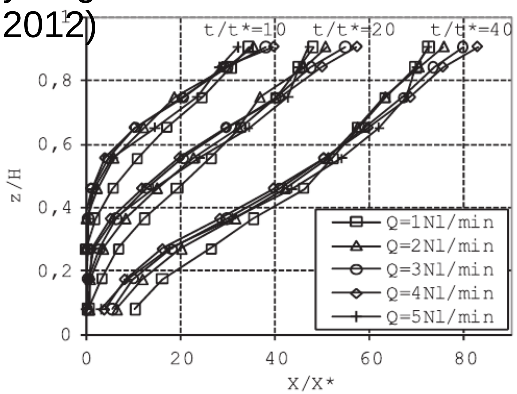
1. Introduction

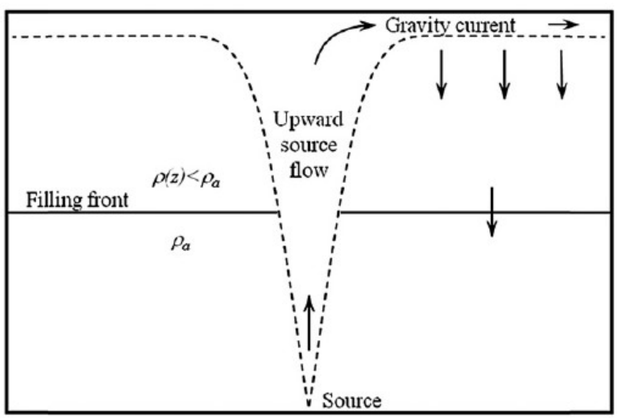


Experiments



Cariteau et al. (Int J Hydrogen Energ, 2012)





Linear profile

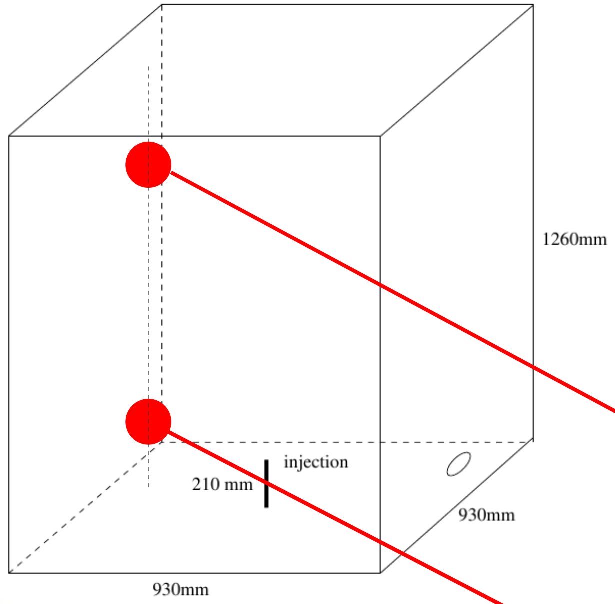
Theoretical models

Baines and Turner (JFM, 1969), Worster and Huppert (JFM, 1983), Cleaver et al. (J. Hazard. Mater., 1994) :

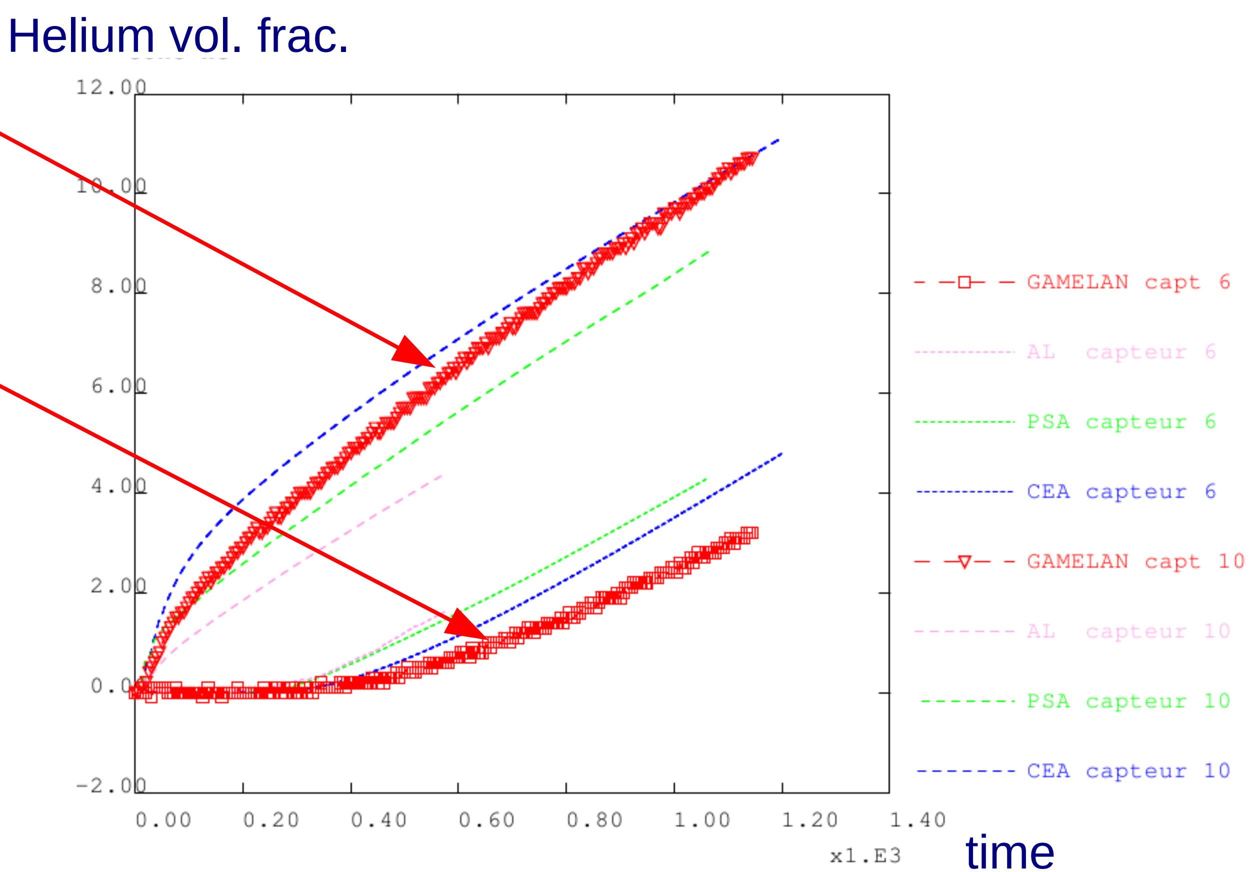
parabolic profile of concentration

Entrainment coefficient α ?

Benchmark of helium-air dispersion (CEA) : evaluate numerical codes



- Comparison of numerical results and experimental data : large discrepancies in low injection case!



- Experimental results : agree with theoretical model

  Bernard-Michel et al. (Technical Report, 2012), Cariteau et al. (Int J Hydrogen Energ, 2012)

Present study

Objective

- Develop a 2D numerical tool to simulate the mixing and dispersion a binary mixture of helium and air in a cavity

Method

- Use DNS with axisymmetric hypothesis
- Validate the results with an incompressible test case of Rogers & Morris, Phys. Fluids, 2009
- Compare numerical results with the model of Worster & Huppert, JFM, 1983
- Compare numerical results with other numerical and experimental data

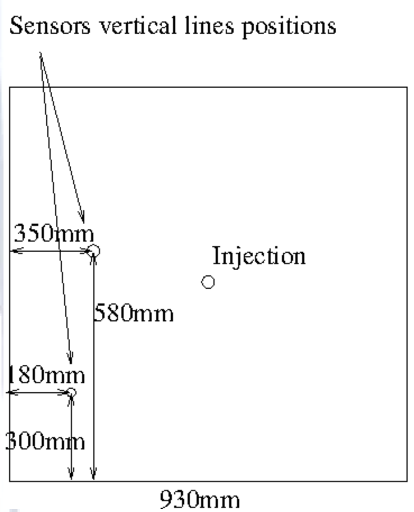
2. Configuration

Experimental vs. Numerical

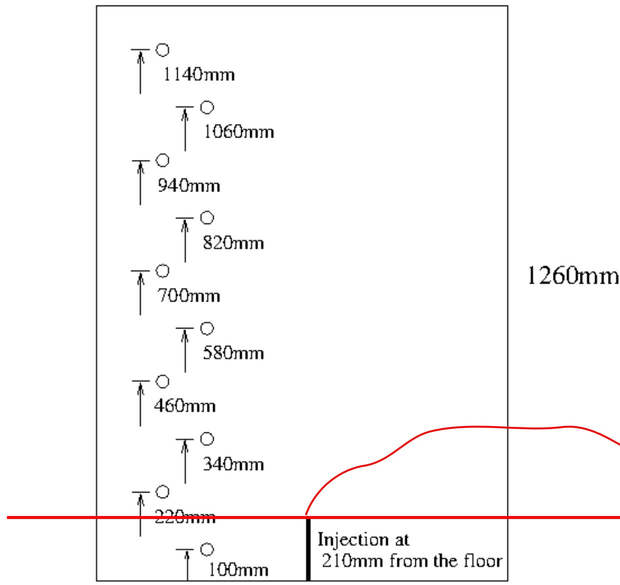
- T=20^{o}C, P = 1 atm
- Ambient fluid : air, injected fluid : helium

GAMELAN : 3D rectangular parallelepiped

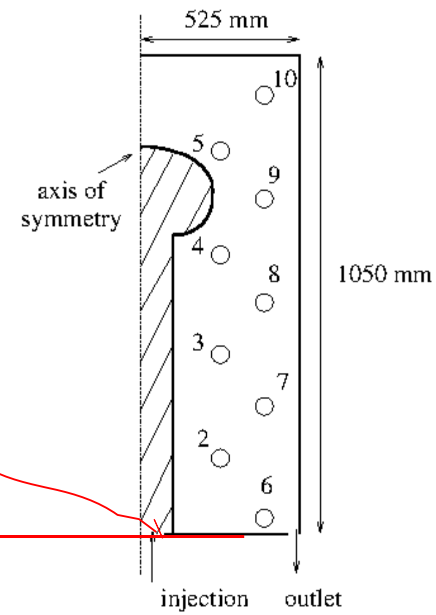
[Num] : 2D axisymmetric

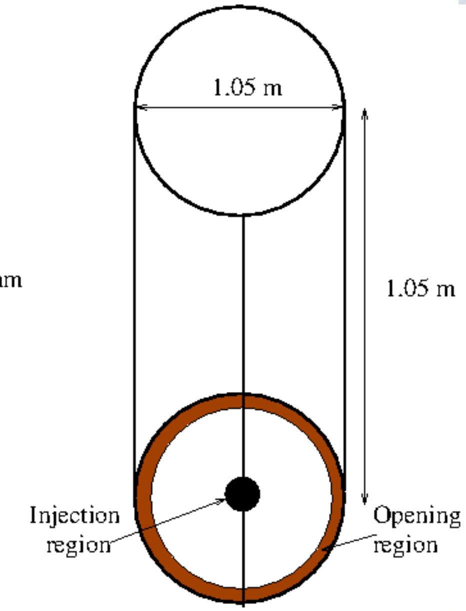


Top view



Side view





Physical parameters of 5 cases

- Physical properties of air and helium

ρ_i $[kg/m^3]$	Y_i [-]	ρ_a $[kg/m^3]$	Y_a [-]	$\frac{\Delta\rho}{\rho_a}$ [-]	ν_i $[m^2/s]$	ν_a $[m^2/s]$	D $[m^2/s]$
0.164	1	1.184	0	0.862	$11.7 \cdot 10^{-5}$	$1.51 \cdot 10^{-5}$	$6.93 \cdot 10^{-5}$

- 4 cases of smaller cavities

Cavity	Gr	d_i/d	Ri_v
1/10	4.3×10^7	0.19	0.15
1/5	3.4×10^8	0.1	1.16
2/5	2.7×10^9	0.05	9.28
3/5	9.3×10^9	0.03	31.3
1	3.7×10^{10}	0.02	145

- Grashof $Gr = g\frac{\Delta\rho}{\rho_a}\frac{H^3}{\nu_a^2}$
- Volume Richardson $Ri_v = g\frac{\Delta\rho}{\rho_i}\frac{V^{1/3}}{{w_i}^2}$
- Schmidt = 0.218 ($Sc_a = \frac{\nu_a}{D_a}$)
- Injection Reynolds = 39. 3

($Re_i = \frac{w_i d_i}{\nu_i}$)

3. Physical modeling

Equations for a binary mixture at constant temperature and pressure

$$
\begin{aligned}
\nabla \cdot \mathbf{u} &= \frac{1}{ReSc_a}(\epsilon_M - 1)\nabla \cdot (\rho \nabla Y) \\
\frac{\partial \rho Y}{\partial t} + \nabla \cdot (\rho Y \mathbf{u}) &= \frac{1}{ReSc_a}\nabla \cdot (\rho \nabla Y) \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) &= -\nabla p + \frac{1}{Re}\nabla \cdot (\rho \nu (\nabla \mathbf{u} + \nabla^t \mathbf{u})) + \frac{1}{Fr}\rho \mathbf{z} \\
\rho &= \frac{1}{1 + (\epsilon_M - 1)Y}
\end{aligned}
$$

+ Laws for the variation ν with Y

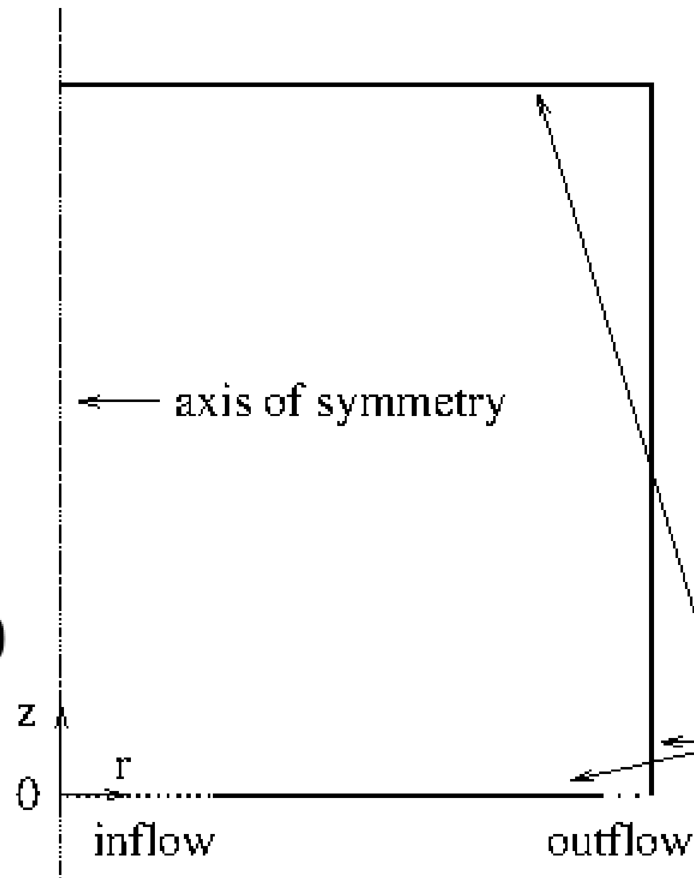
- Y : helium mass fraction, ρ : mixture density
- $\mathbf{u}$: mass-averaged velocity, $\epsilon_M = M2/M1 = 7.24$
- $Re = \dfrac{w_i H}{\nu_a}$, $Fr = \dfrac{w_i^2}{gH}$, $X = \dfrac{\epsilon_M Y}{1 + (\epsilon_M - 1)Y}$

Boundary conditions

$$\frac{\partial u}{\partial r} = 0$$

$$\frac{\partial w}{\partial r} = 0$$

$$\frac{\partial Y}{\partial r} = 0$$



$$\frac{\partial Y}{\partial r} = 0$$

$$u = 0$$

$$w = 0$$

$$Y = \overline{Y_i} \quad u = 0 \quad w = \overline{w_i}$$

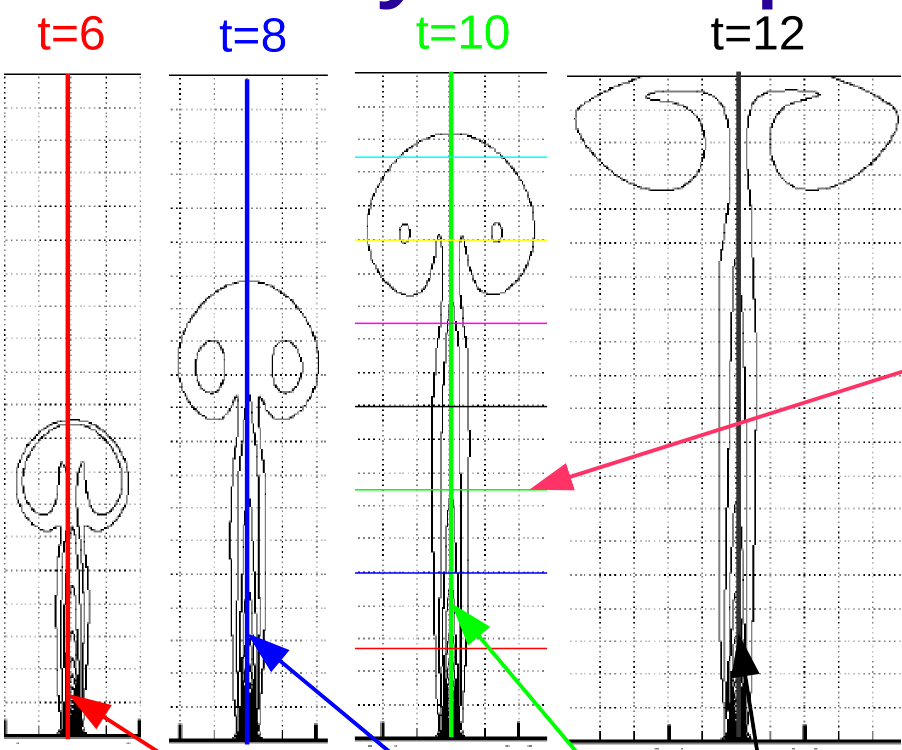
$$\frac{\partial Y}{\partial \mathbf{n}} = 0 \quad u = 0 \quad \frac{\partial w}{\partial z} = 0$$

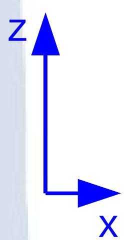
4. Numerical methods and validation

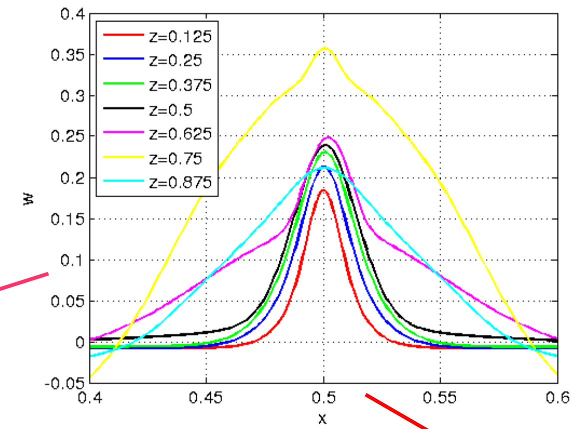
Numerical methods

- Time discretization : Semi-implicit, 2nd order
- Spatial discretization : finite volume, staggered grid, 2nd order
- Non-uniform grid with 322x642 nodes for the full cavity
- Time to simulate 275 s (physical time) for the full cavity : 1228.5 hours (CPU time)

2D cavity : comparison with theory

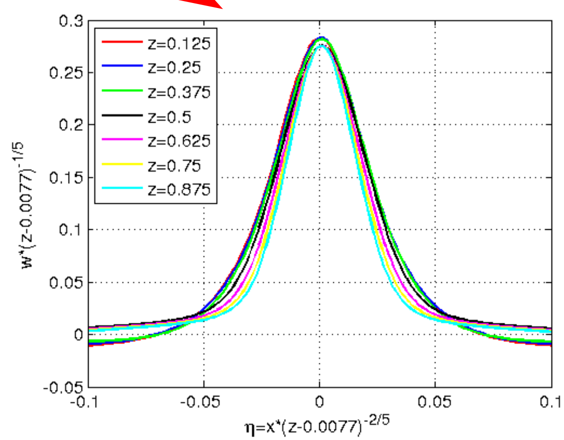




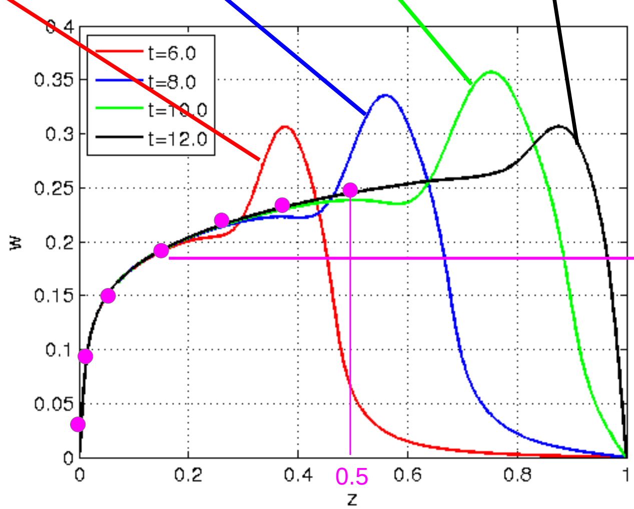


Horizontal profile of w

change of variables



Centerline profile of w



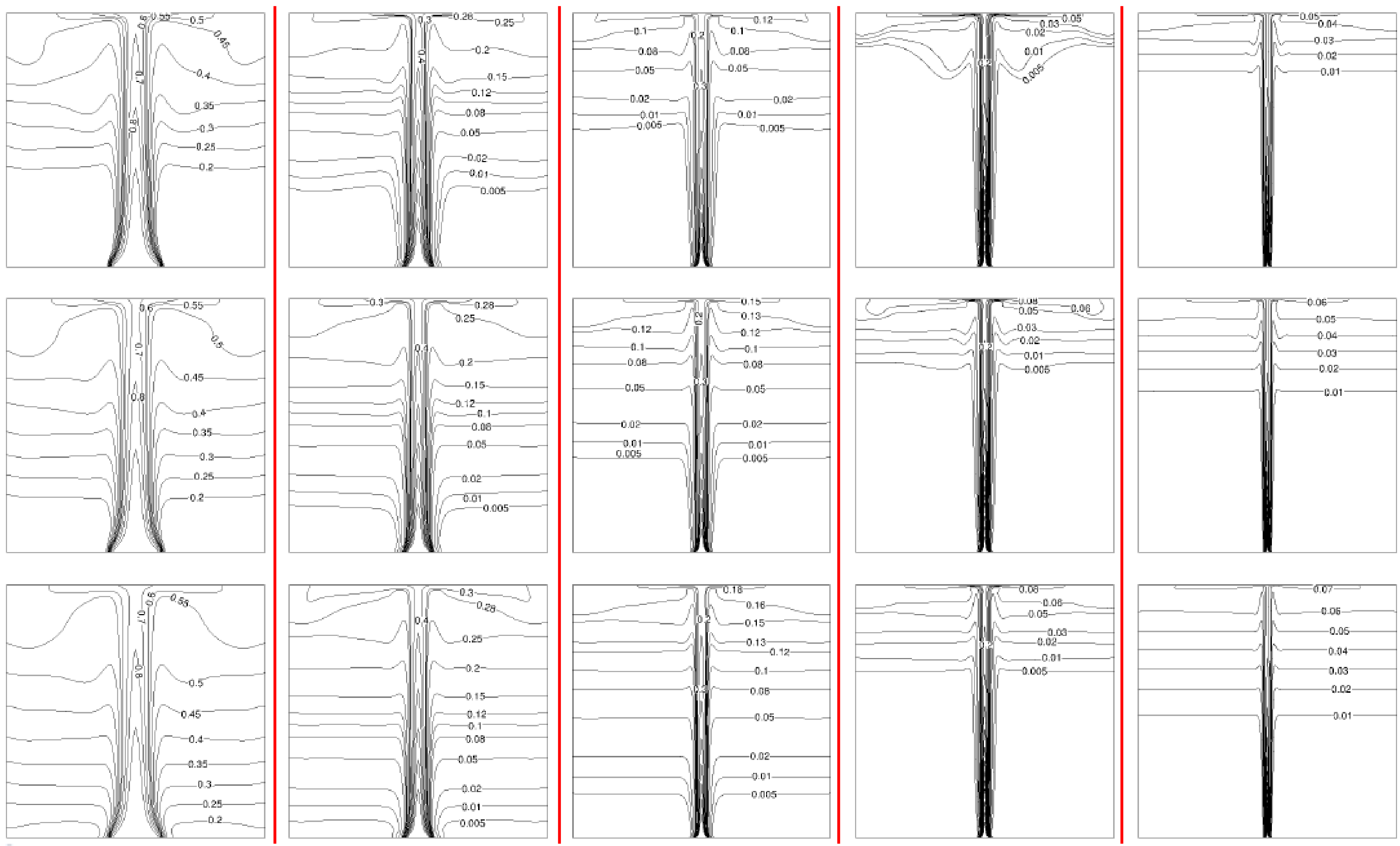
$$w_c(z) = 0.2835(z - 0.0077)^{1/5}$$

$$\rho_a - \rho_c(z) = 0.002(z - 0.0073)^{-3/5}$$

5. Results of round plumes with axisymmetric assumption

Volume fraction fields

time



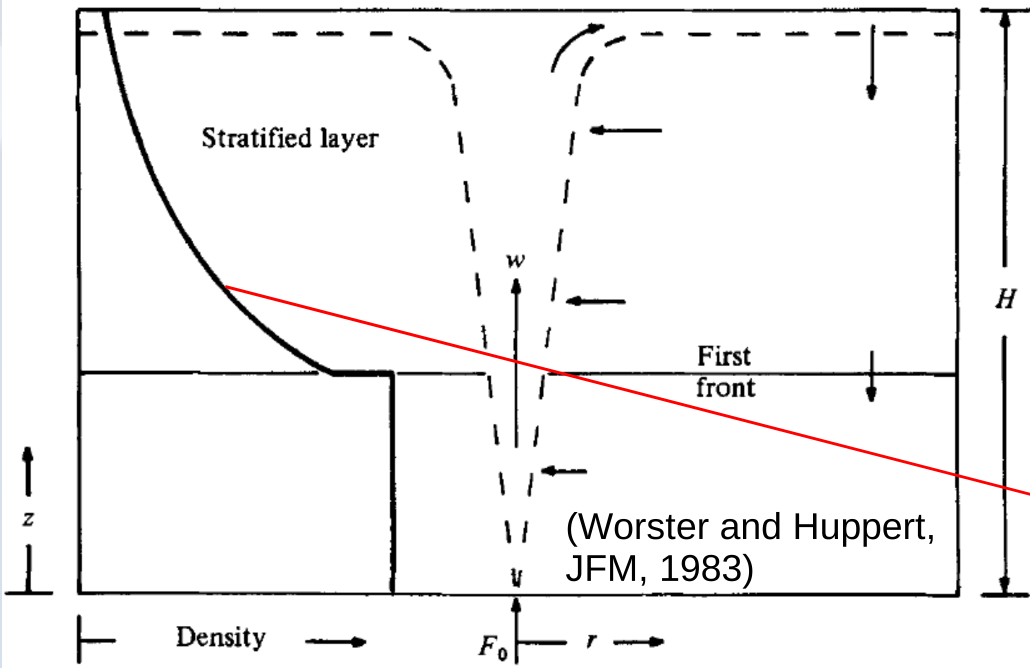
Cavity 1/10 | Cavity 1/5 | Cavity 2/5 | Cavity 3/5 | Cavity 1

Volume fraction profile : Worster and Huppert's model

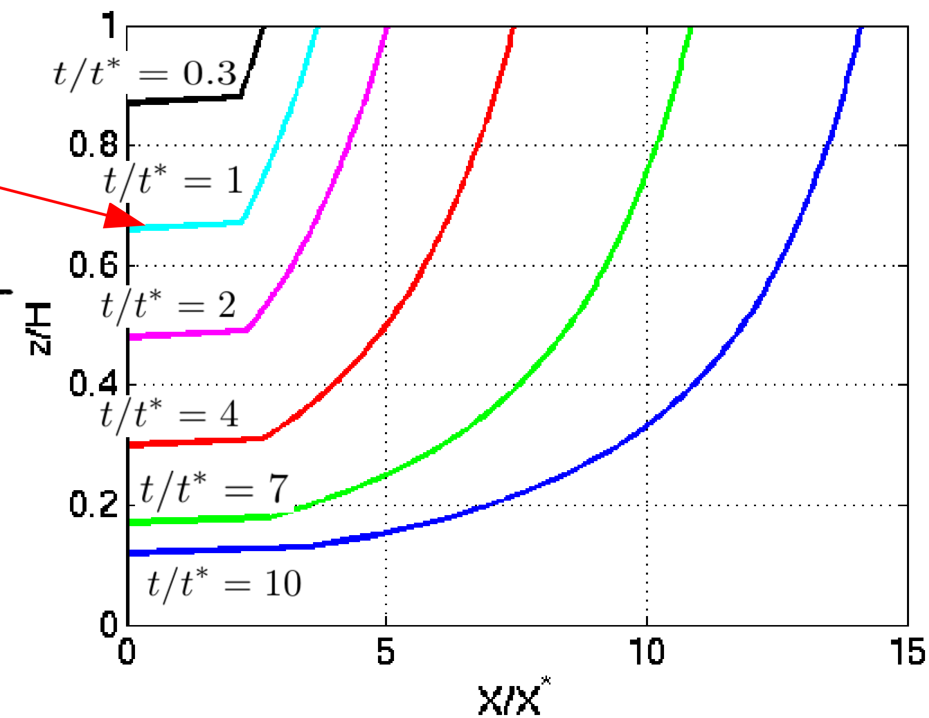
- During the descend of the first front

$$t^* = \frac{A}{4\pi^{2/3}\alpha^{4/3}H^{2/3}B_0^{1/3}}$$

$$X^* = \frac{B_0^{2/3}}{4\alpha^{4/3}H^{5/3}g\frac{\rho_a-\rho_i}{\rho_a}}$$



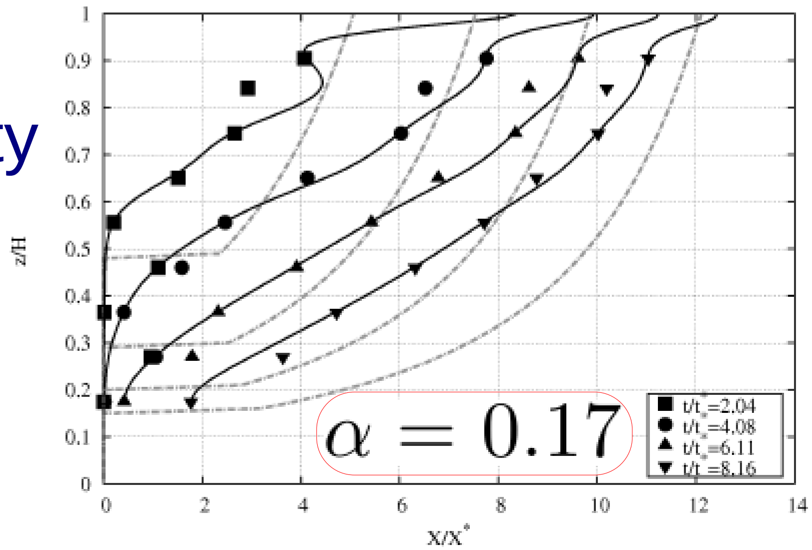
(Worster and Huppert, JFM, 1983)



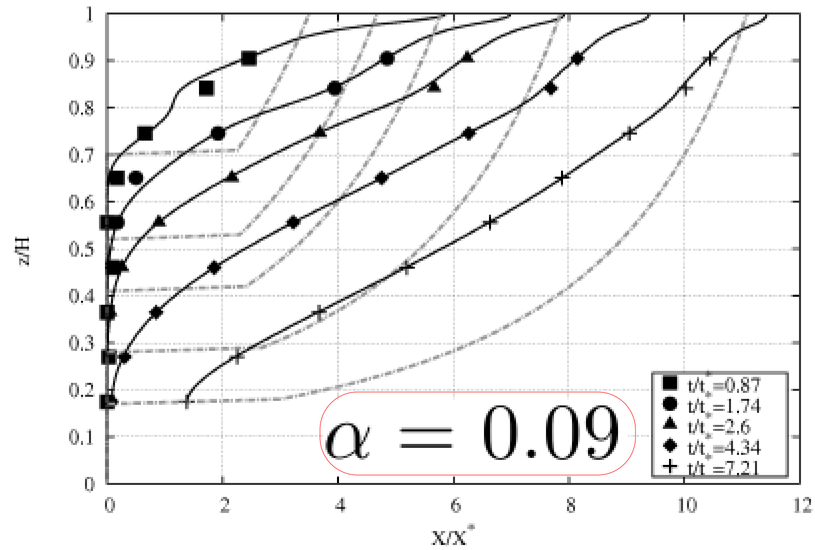
- Source buoyancy flux : $B_0 = g\frac{\rho_a - \rho_i}{\rho_a}$
- Cross-sectional area : A
- Entrainment coefficient : α

Volume fraction profile : comparison with Worster and Huppert's model

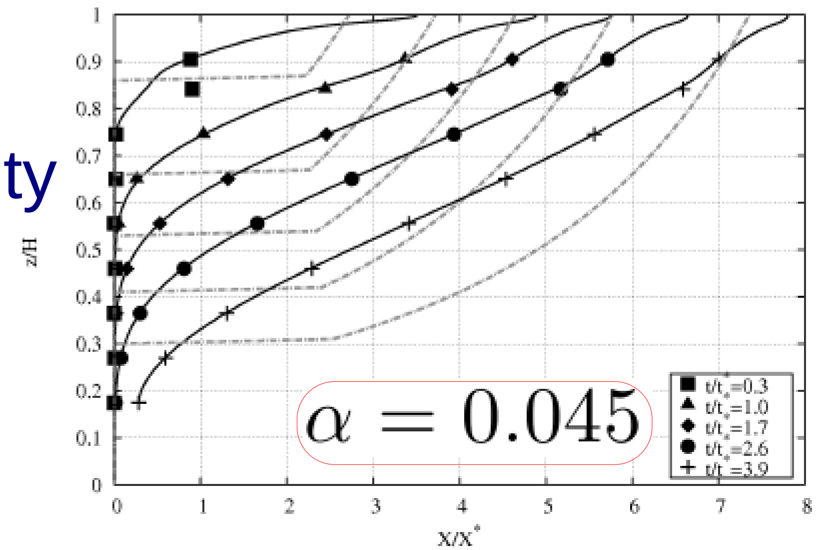
Cavity 1/10



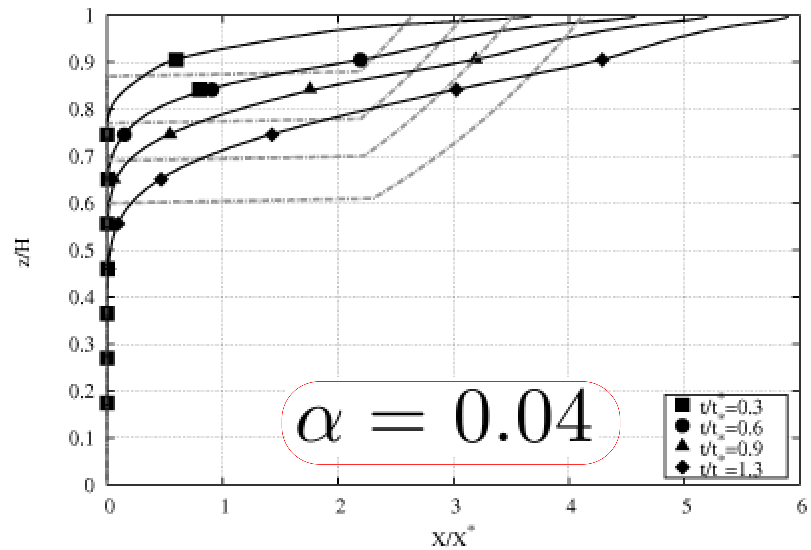
Cavity 1/5



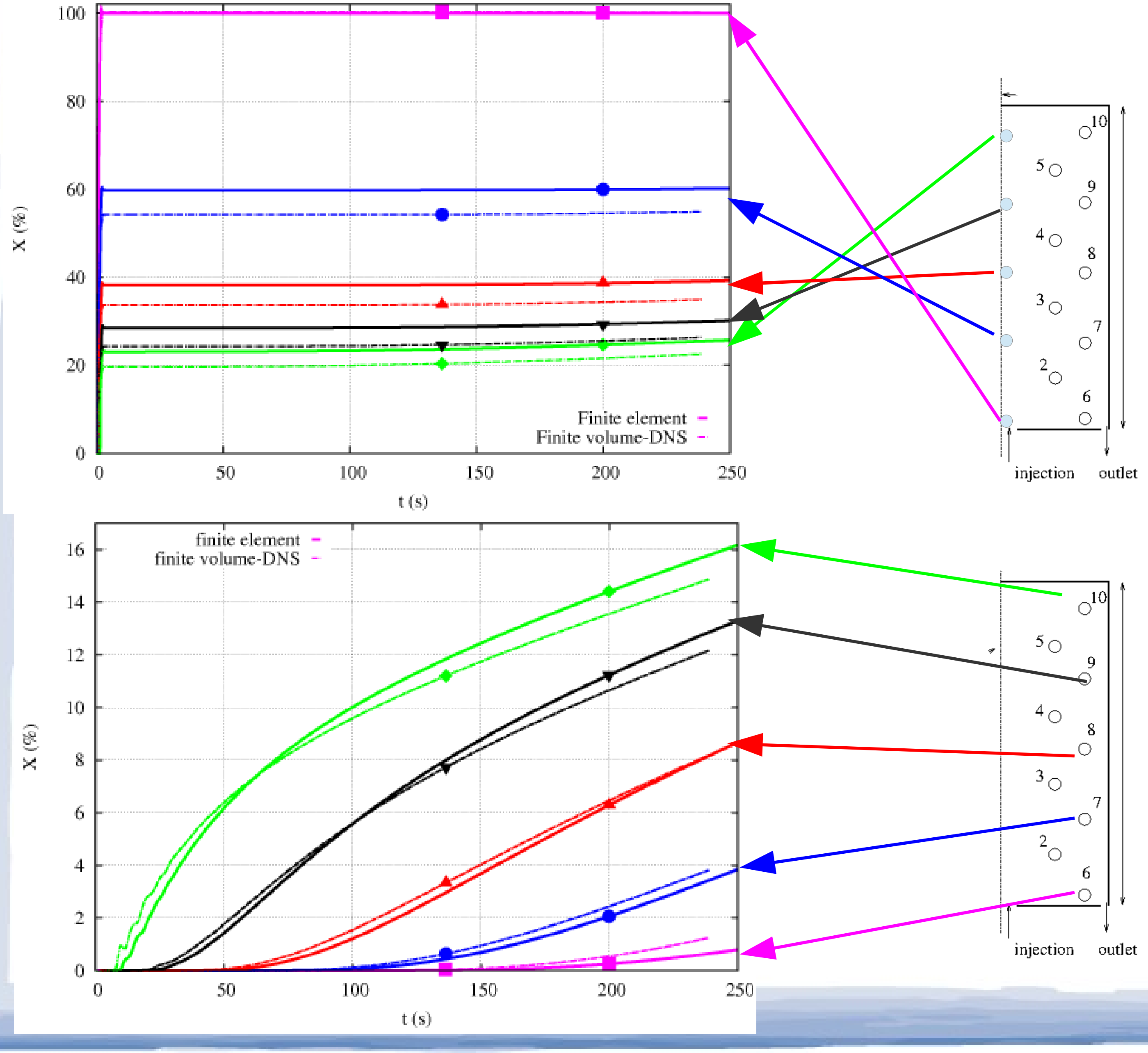
Cavity 2/5



Cavity 3/5



Volume fraction : comparison with finite element results for cavity 3/5



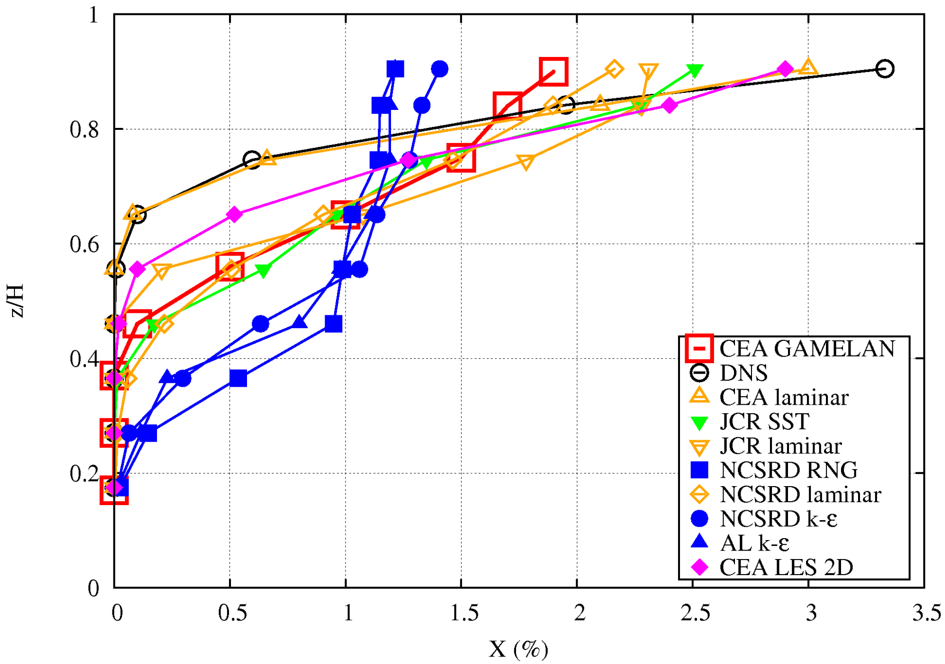
- at 5 points on axis

Same axisymmetric assumption

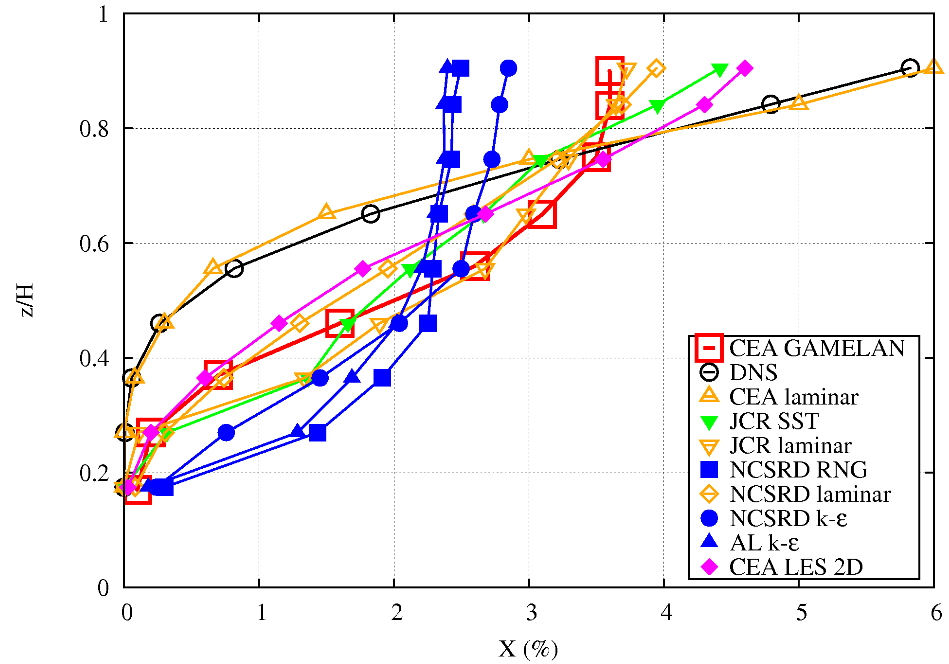
- at 5 points off axis

Comparison for the full cavity

115 s



275 s



- CEA laminar, JCR laminar, NCSRD laminar : no turbulence model
- CEA LES 2D : LES with axisymmetric hypothesis
- NCSRD RNG, NCSRD $k-\epsilon$, AL $k-\epsilon$: $k-\epsilon$ model
- JCR SST : $k-\omega$ model
- Data taken from Bernard-Michel (Proceedings ICHS, 2013)

Conclusions and perspectives

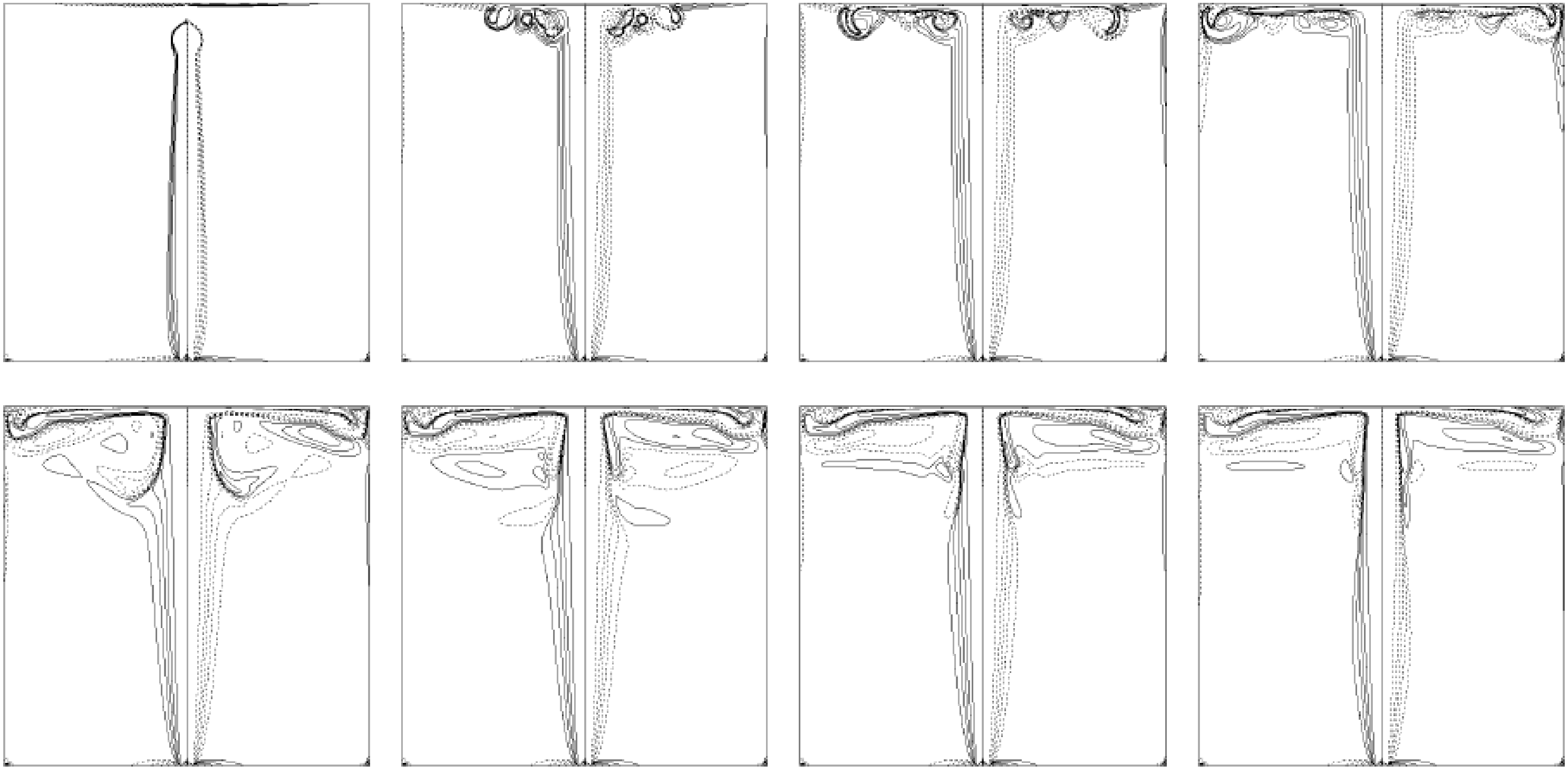
- Develop a numerical tool to simulate the dispersion and mixing of helium injected in an air-filled cavity with axisymmetric hypothesis
- Validate the 2D plane case with theory
- Five cavities with the same aspect ratio have been investigated
- Obtain close agreement with finite element results with the same axisymmetric assumption
- The numerical results do not agree with either Worster and Huppert's model or experimental data

  ---> The need to perform full 3D computations

References

- [1] M. G. Worster and H. E. Huppert (1983) *Time-dependent density profiles in a filling box*. J. Fluid Mech. 132
- [2] B. Cariteau and I. Tkatschenko (2012) *Experimental study of the concentration build-up regimes in an enclosure without ventilation.* International Journal of Hydrogen Energy 37
- [3] W. D. Baines and J. S. Turner (1969) *Turbulent buoyant convection from a source in confined region*. J. Fluid Mech. 37(1) 51-80
- [4] R. P. Cleaver and M. R. Marshall and P. F. Linden (1994) *The build-up of concentration within a single enclosed volume following a release of natural gas*. J. Hazard. Mater. 36 209-226
- [5] M. C. Rogers and S. W. Morris (2009). *Natural versus forced convection in laminar starting plumes*. Physics of Fluids, 21.
- [6] G. Bernard-Michel, J. Trochon, E. Vyazmina and O. Gentilhomme (2012) *Resultat du benchmark ventilation sur 3 essais gamelan dans le cadre du projet anr dimitrhy*. Technical Report DEN/DANS/DM2S/STMF/LIEFT/RT/12/020/A., CEA Saclay DEN/DANS/DM2S/STMF/LIEFT.
- [7] G. Bernard-Michel (2013). *CFD benchmark based on experiments of heliume dispersion in a 1 m3 enclosure-intercomparisons for plumes and buoyant jets*. Proceedings of ICHS 2013.

Vorticity fields



- Cavity 3/5, t=4, 10, 20, 46, 93, 139 and 260