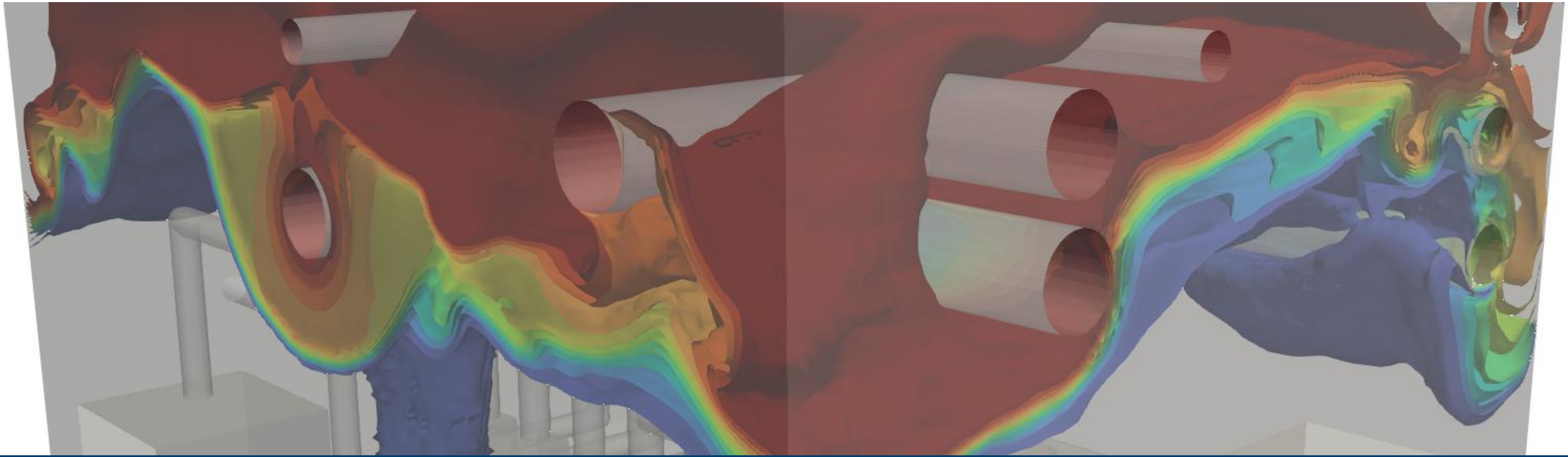


TOWARDS THE SIMULATION OF HYDROGEN LEAKAGE SCENARIOS IN CLOSED BUILDINGS USING CONTAINMENTFOAM

19. SEPTEMBER 2023 I **KHALED YASSIN**, STEPHAN KELM, AND ERNST-ARNDT REINECKE

INTERNATIONAL ASSOCIATION FOR HYDROGEN SAFETY

International Conference on Hydrogen Safety

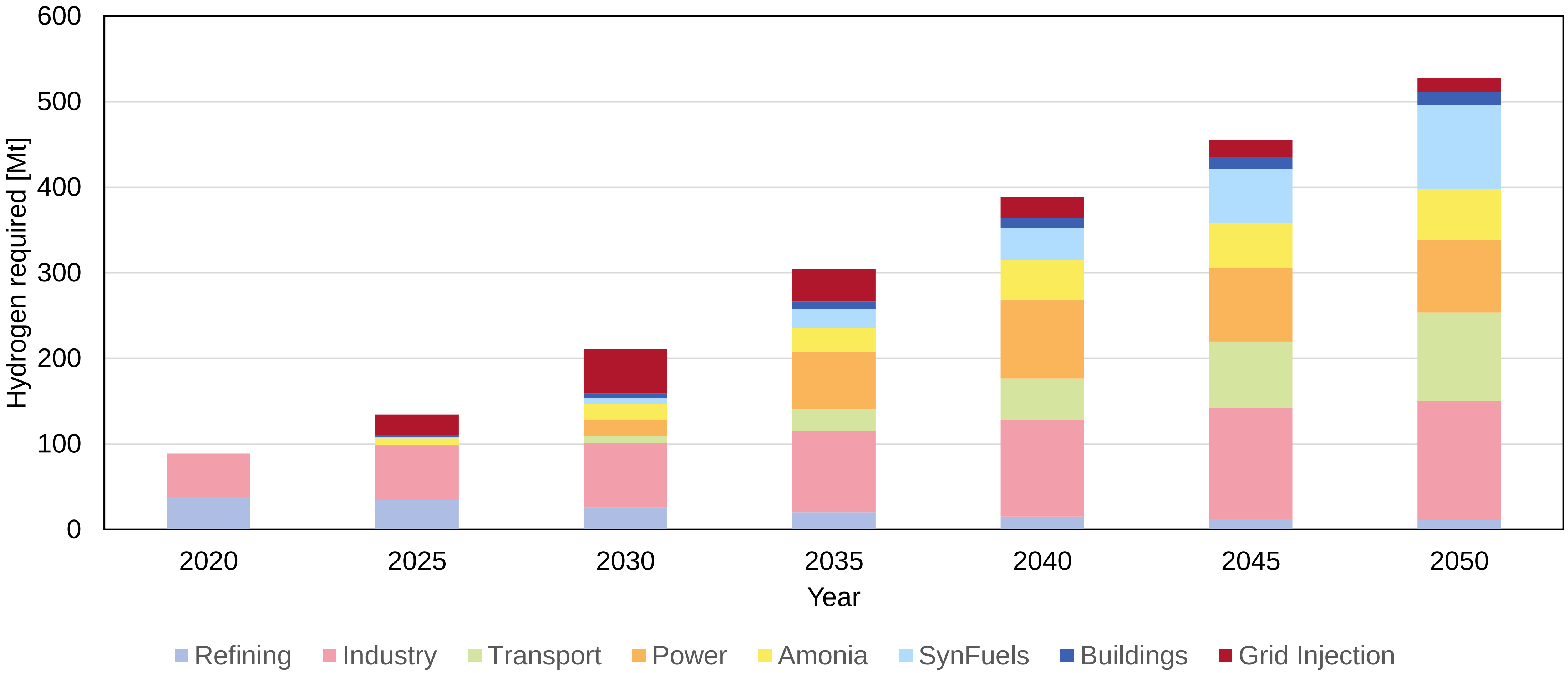
Mitglied der Helmholtz-Gemeinschaft

JÜLICH Forschungszentrum

CONTENT

MOTIVATION

Towards Net Zero Carbon by 2050 – the required hydrogen production



IEA Global Hydrogen Review 2021

MOTIVATION

Safety concerns for indoor hydrogen use

Are the current building codes and regulations reliable?

How GH_2 behave in case of leakage?

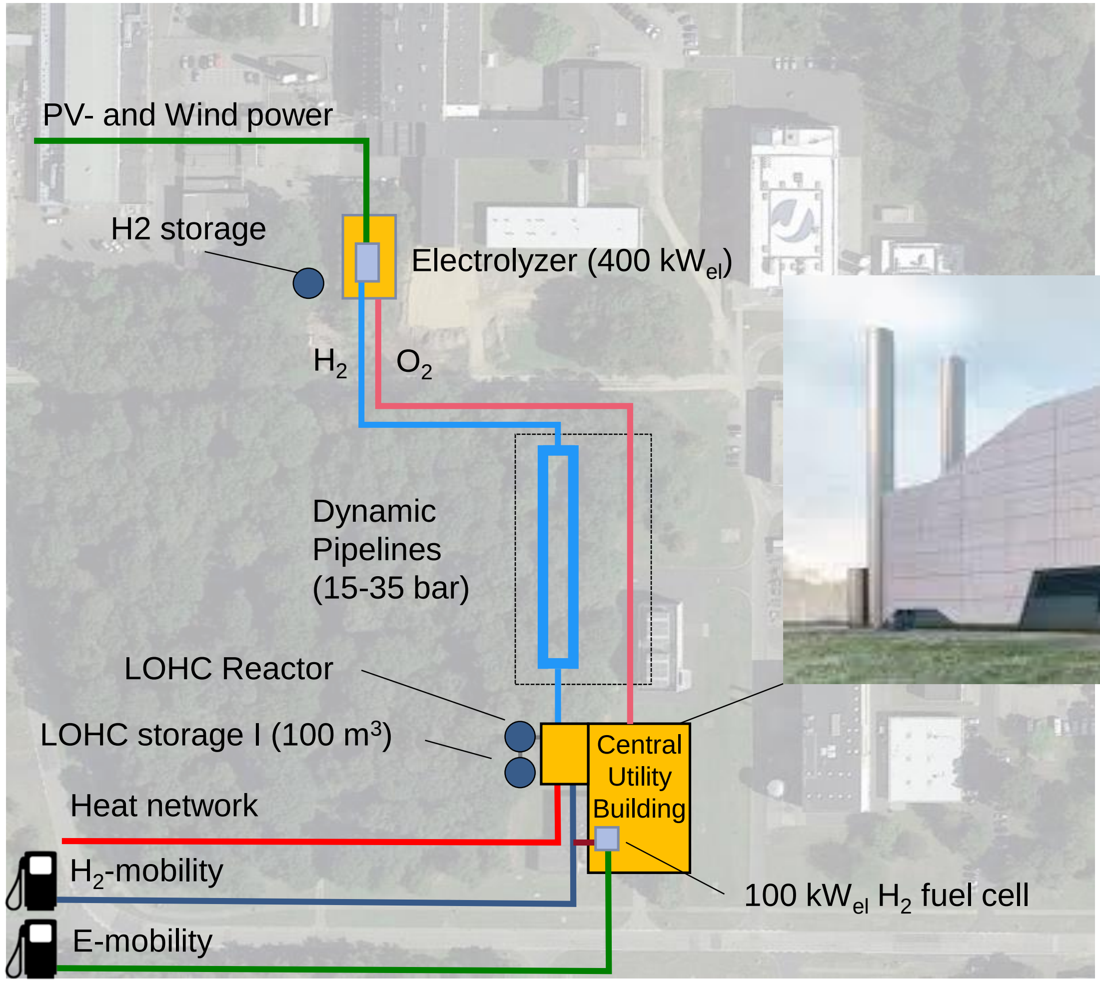
Where to locate the sensors for proper GH_2 detection?

How to extract GH_2 from space in case of leakage?

THE LIVING LAB ENERGY CAMPUS (LLEC) AT FZ JÜLICH

General overview: PtG++ sub project

LOHC
Liquid Organic
Hydrogen Carrier

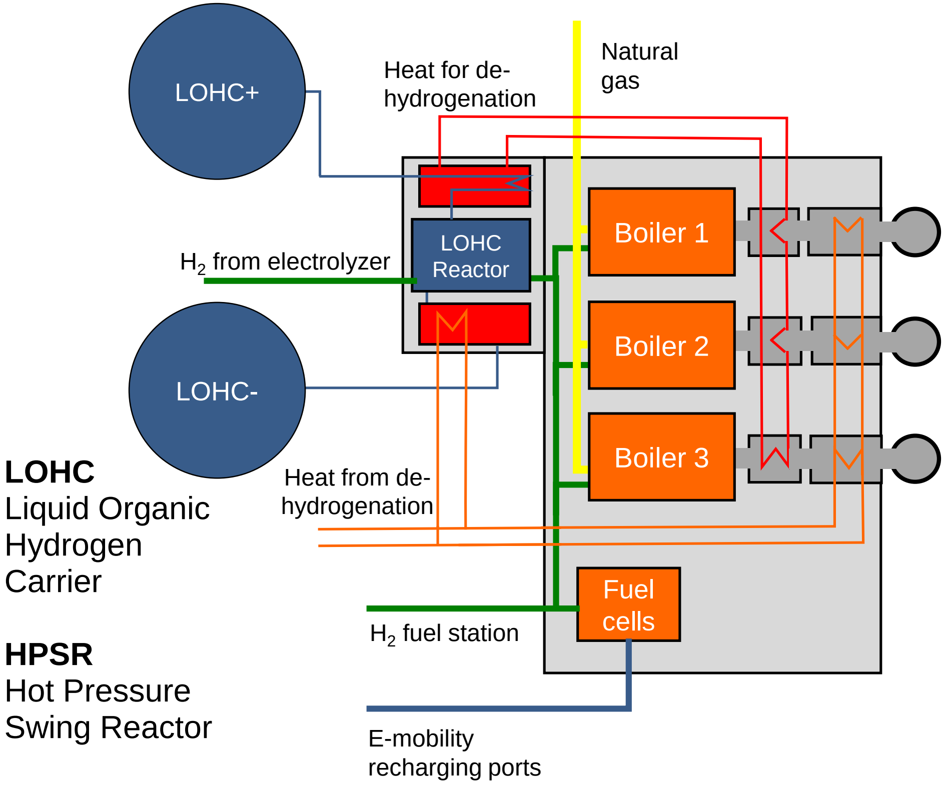


Source: bft Planung GmbH

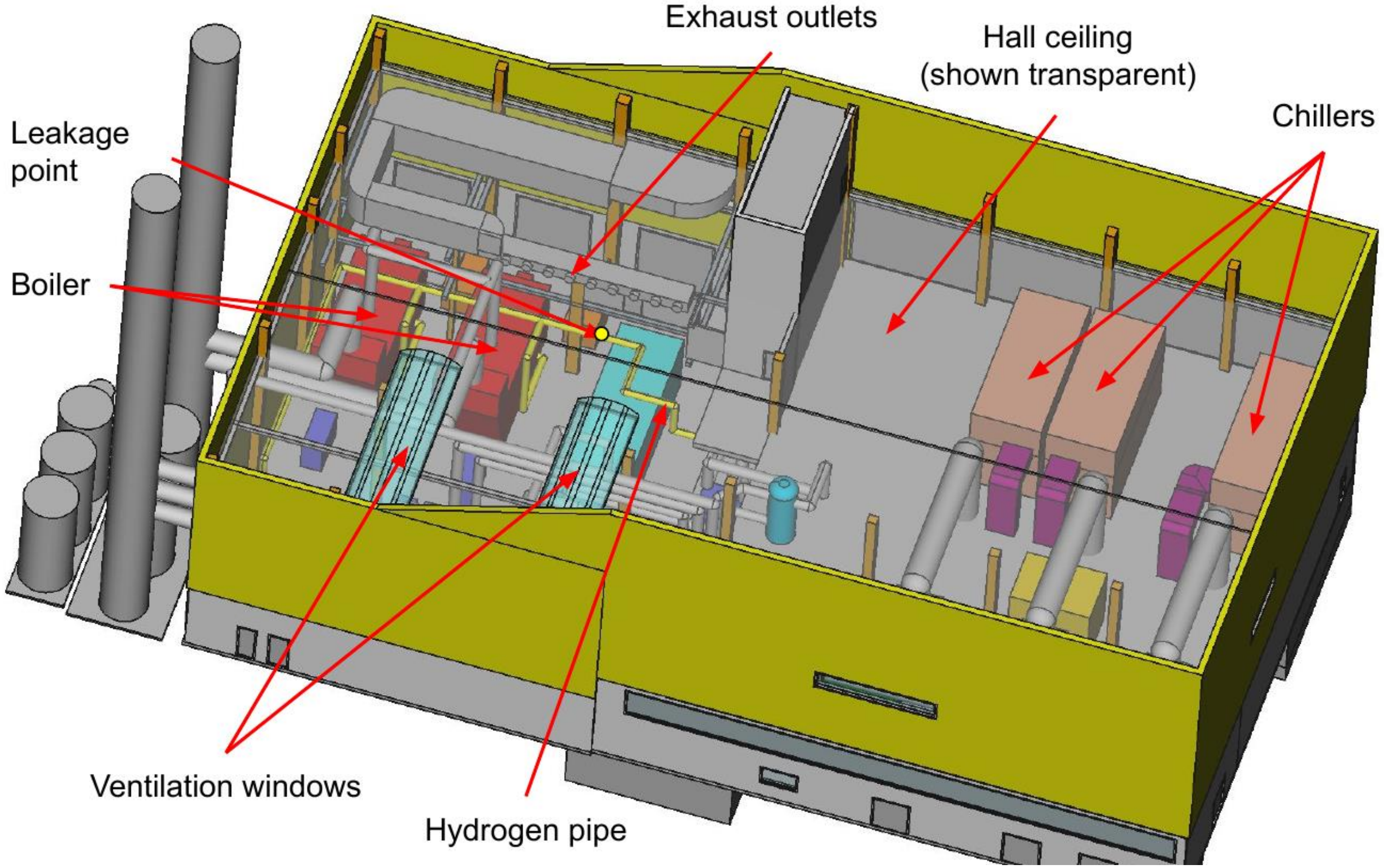
H_2 Cycle in FZ Jülich [S.Kasselmann]

THE LIVING LAB ENERGY CAMPUS (LLEC) AT FZ JÜLICH

The central utility building at Jülich campus



LOHC and Boilers cycle [S.Kasselmann]



Central utility building of FZ Jülich, own figure, 3D CAD Geometry by [C. Newman]

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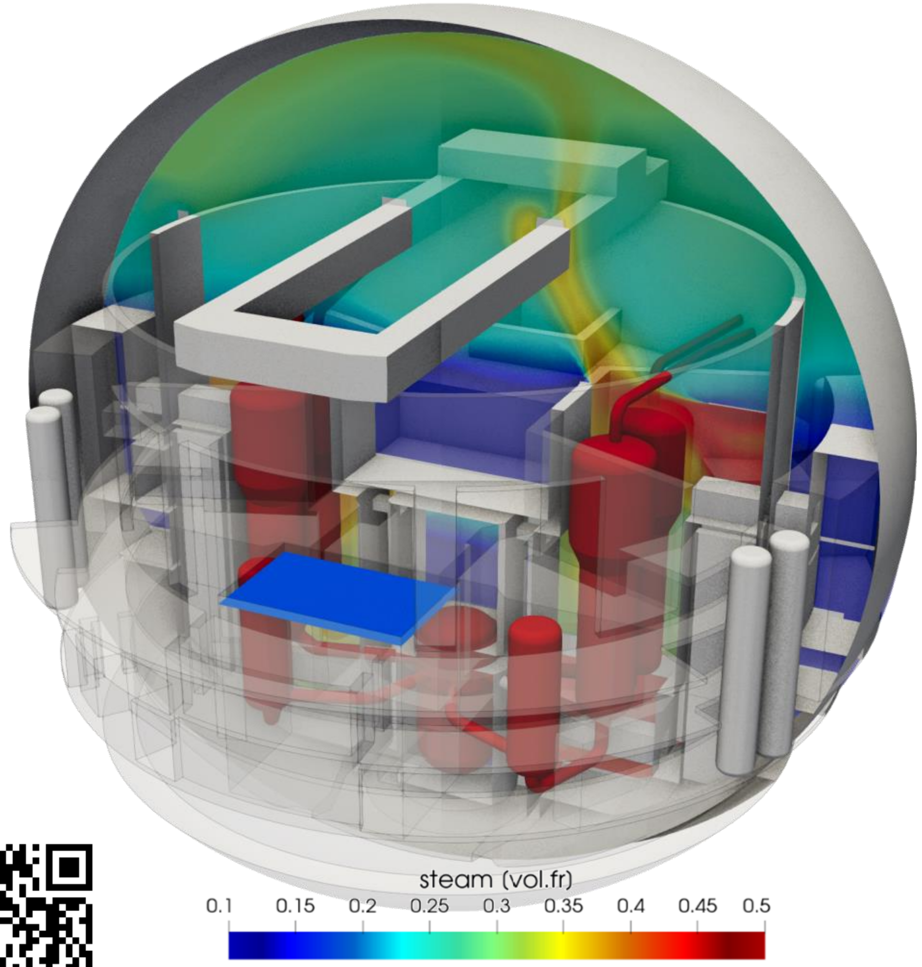
METHODOLOGY

CFD libraries containment∇FOAM

- **Flows and Transport Phenomena [1]**
  - **Efficient Multi-Species Solver:** effective binary diffusion, Wilke mixture
  - **Turbulence transport**: k-ω SST model with buoyancy terms,
  - **PARs:** Code coupling with mechanistic model REKODIREKT
  - **Burst discs, flaps, doors:** conditional mesh interfaces
  - Code coupling with OpenModelica
  - Conjugate heat transfer, Wall condensation, Fog formation, Gas radiation, Aerosol transport, Technical Systems and Components, porous media
- **The codes are extensively validated against different experiments in nuclear and hydrogen applications [2]**

Transferring experience in nuclear safety to hydrogen safety



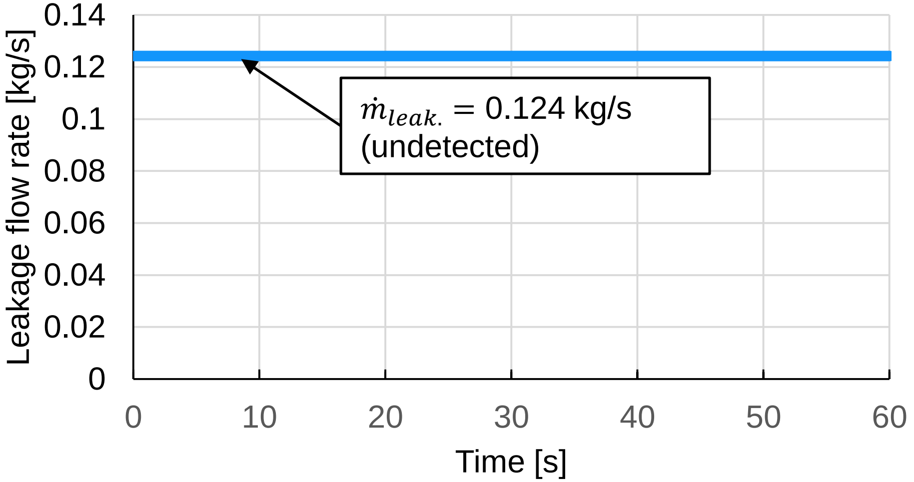
Steam distribution inside the containment, 3D CAD Geometry by [L. Serra-Lopez (UPM)]

[1] Kelm, S. et al. "The Tailored CFD Package 'containmentFOAM' for Analysis of Containment Atmosphere Mixing, H_2/CO Mitigation and Aerosol Transport„ *Fluids* (2021) 6, no. 3: 100.
[2] Yassin, K.; Kelm, S.; Kampili, M.; Reinecke, E.-A. Validation and Verification of containmentFOAM CFD Simulations in Hydrogen Safety. *Energies* **2023**, *16*, 5993. https://doi.org/10.3390/en16165993

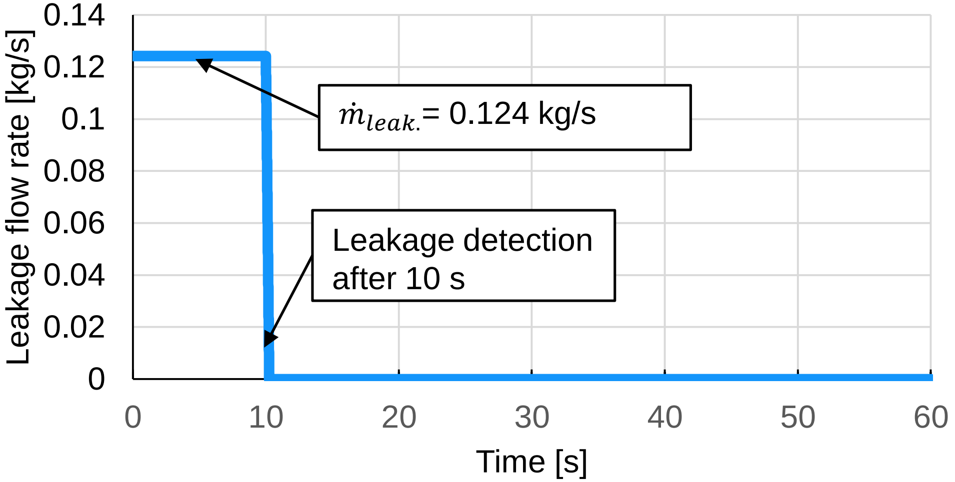
METHODOLOGY

Scenarios

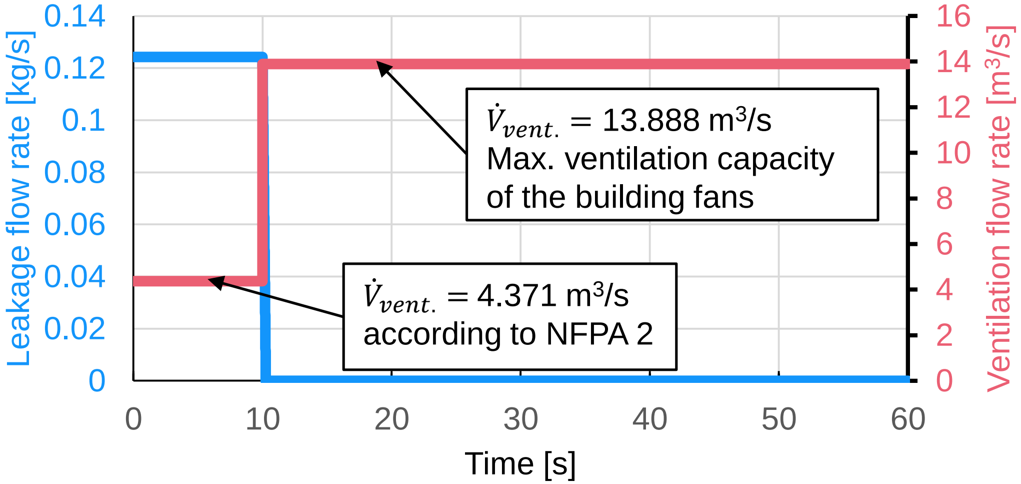
No Ventilation / No detection (Scenario 1)



Natural Ventilation (Scenario 2)



Forced Ventilation (Scenario 3)



METHODOLOGY

Simulation parameters

Flow parameters

$D_{leak.}$= 40 mm
p = 0.6 bar(g)
$T_{amb.}$= 298.15K
$T_{leak.}$= 255.13K
ρ = 0.0959 kg/m^3

Grid parameters

Max. cell volume = 0.55 m^3

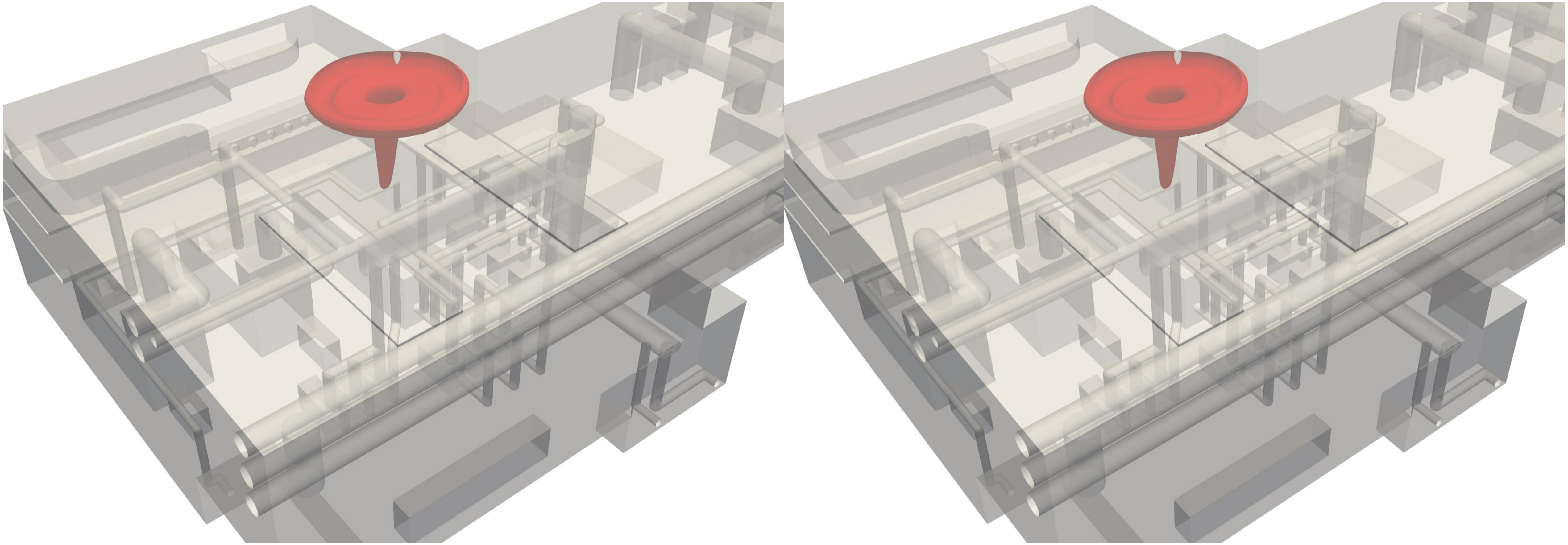
	N_{cells}	V_{domain}
Forced/No Vent.	11.3 Mio.	10,150 m^3
Natural Vent	15.7 Mio.	15,050 m^3

Computational cost

Forced/No Vent.≈ 1130 core-hours / sim. s
Natural Vent. ≈ 6340 core-hours / sim. s
at CFL=0.99

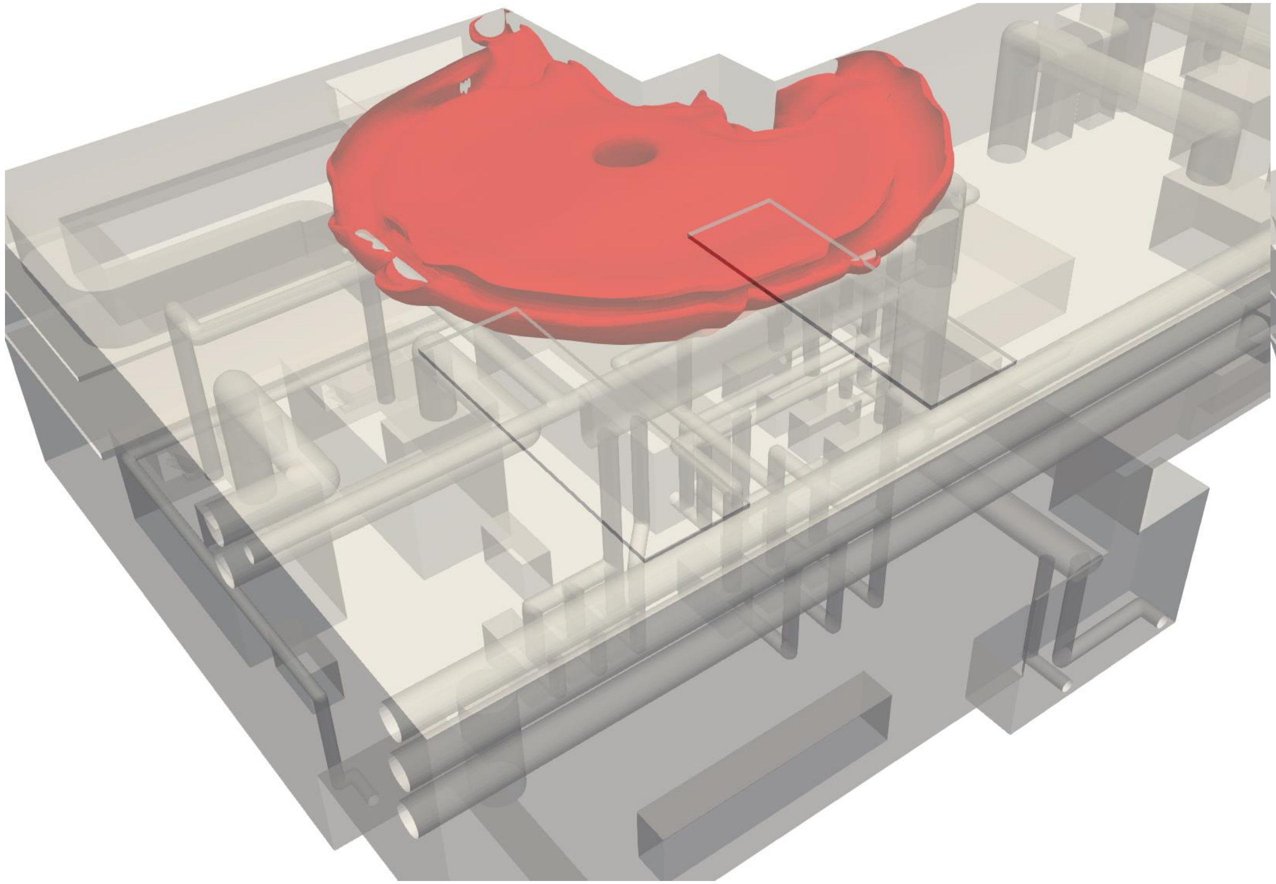
RESULTS

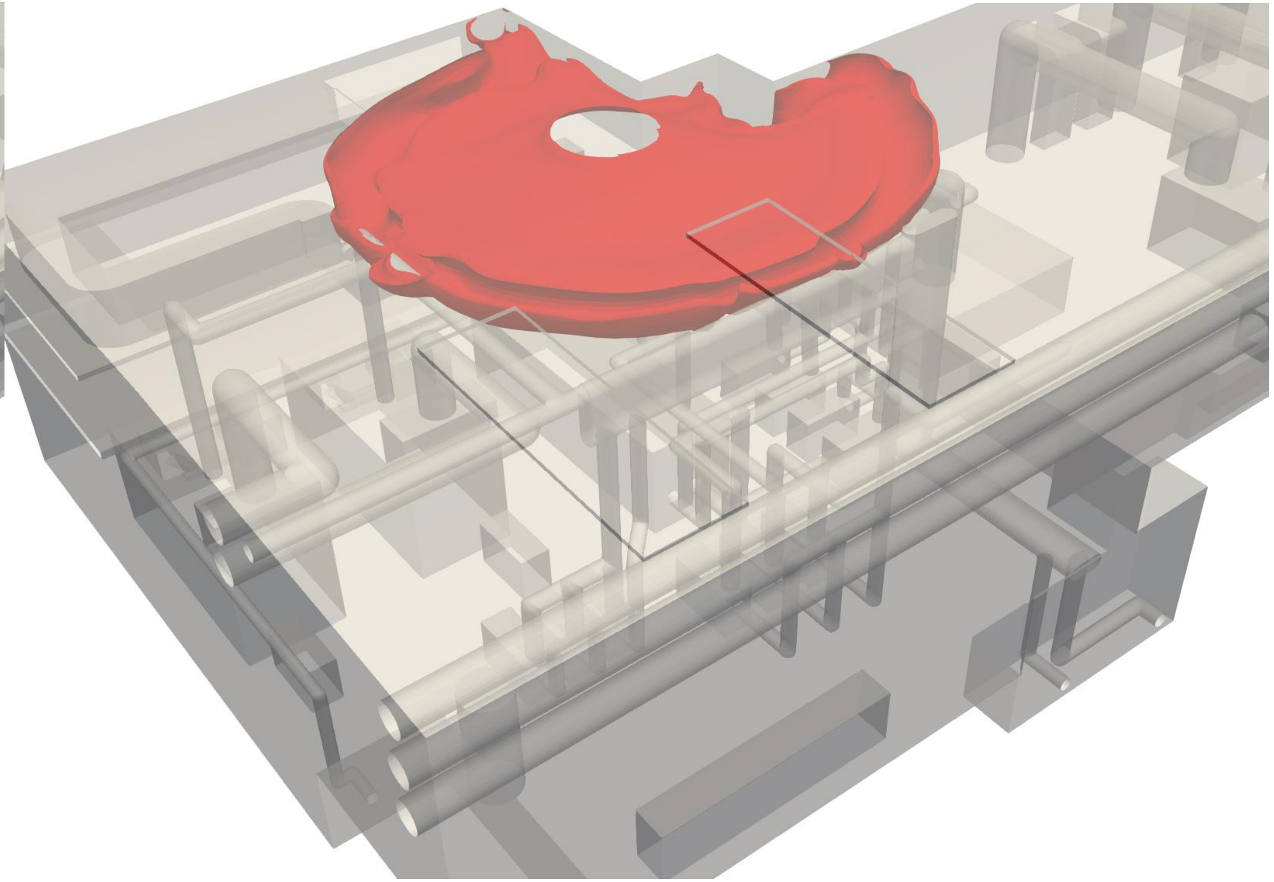
No ventilation vs Mechanical - cloud development (contour surface represents the LFL surface)
After 5 s



RESULTS

No ventilation vs Mechanical
After 15 s

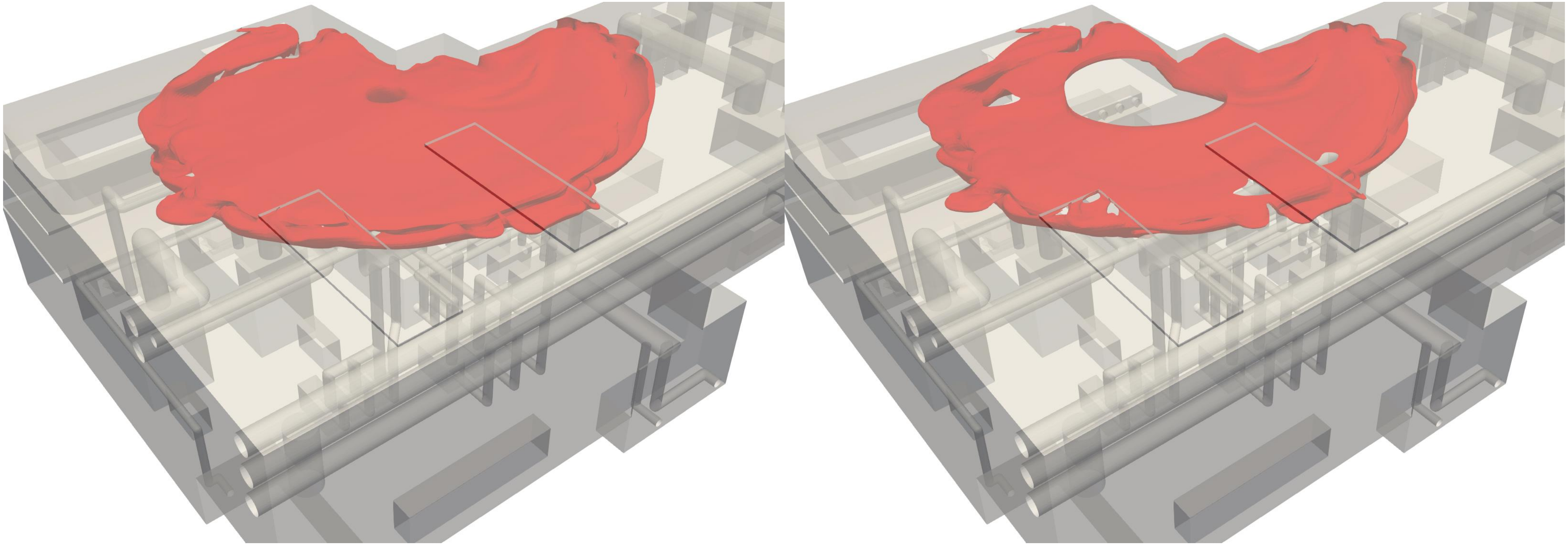




RESULTS

No ventilation vs Mechanical

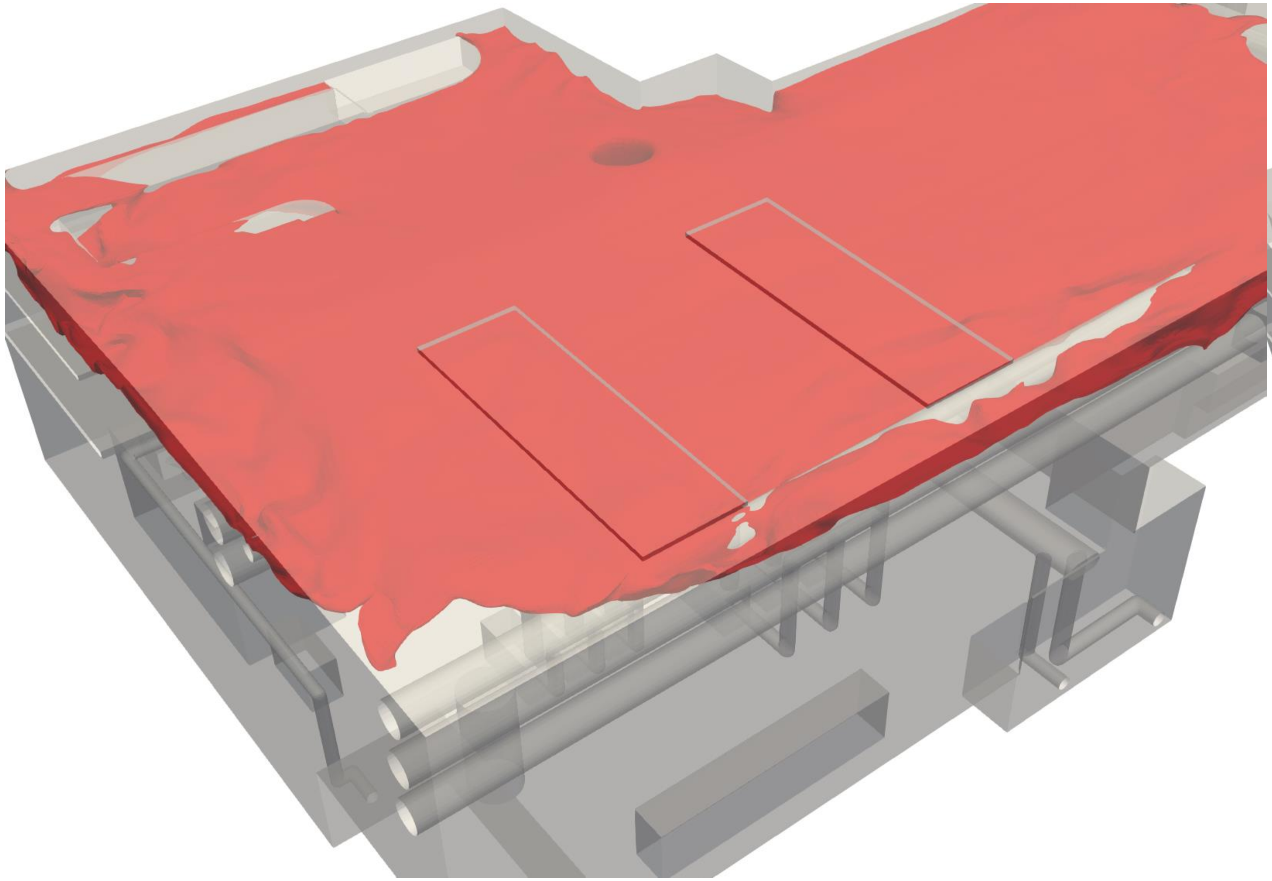
After 20 s

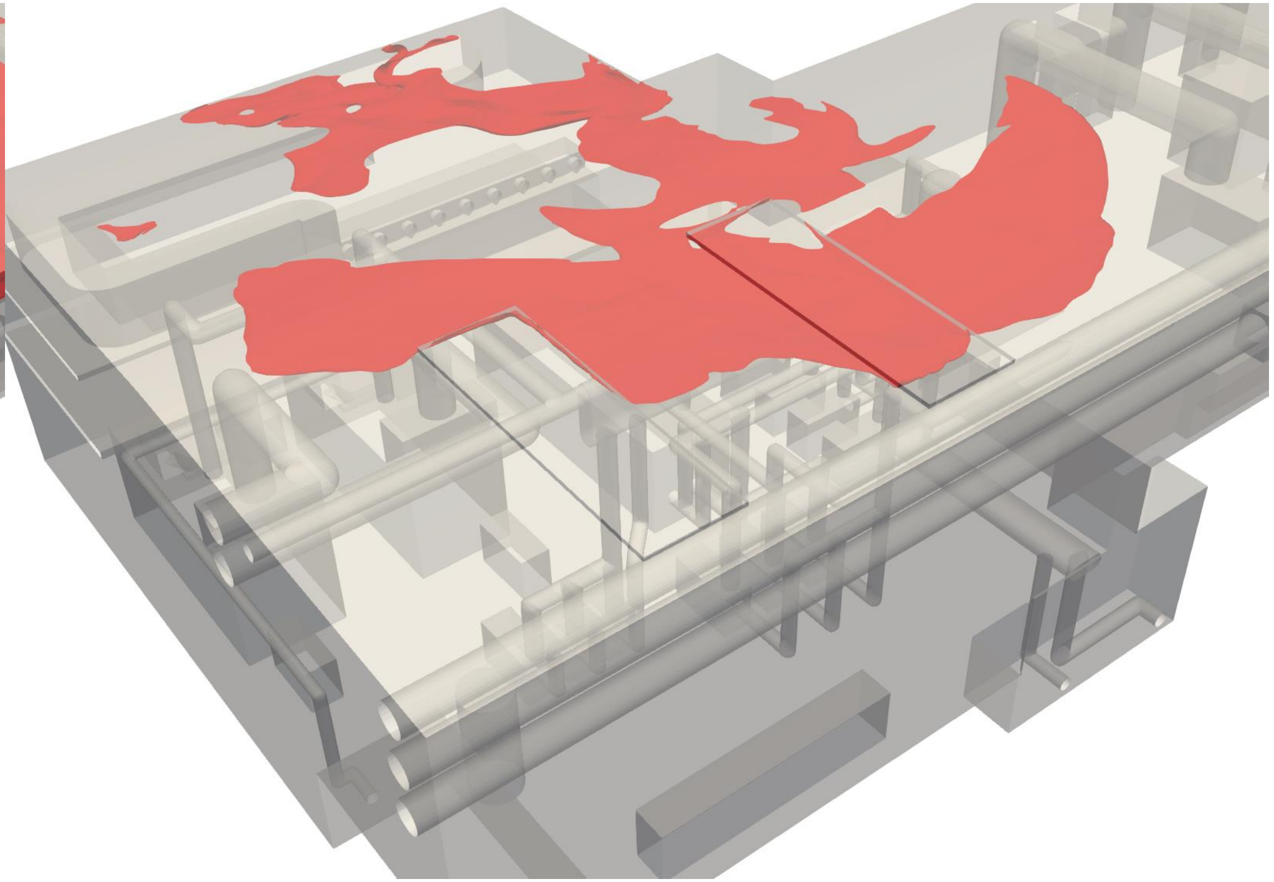


RESULTS

No ventilation vs Mechanical

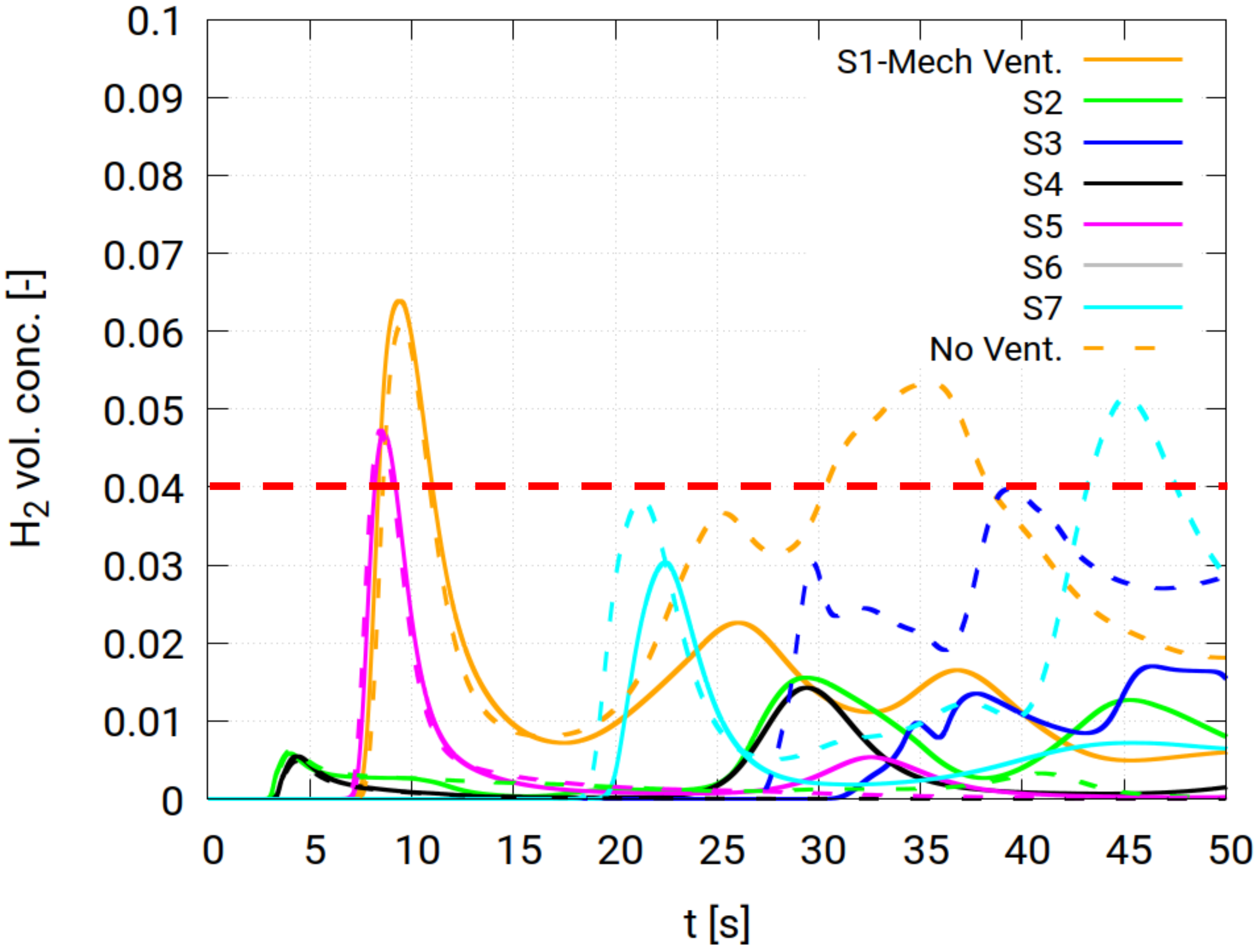
After 40 s

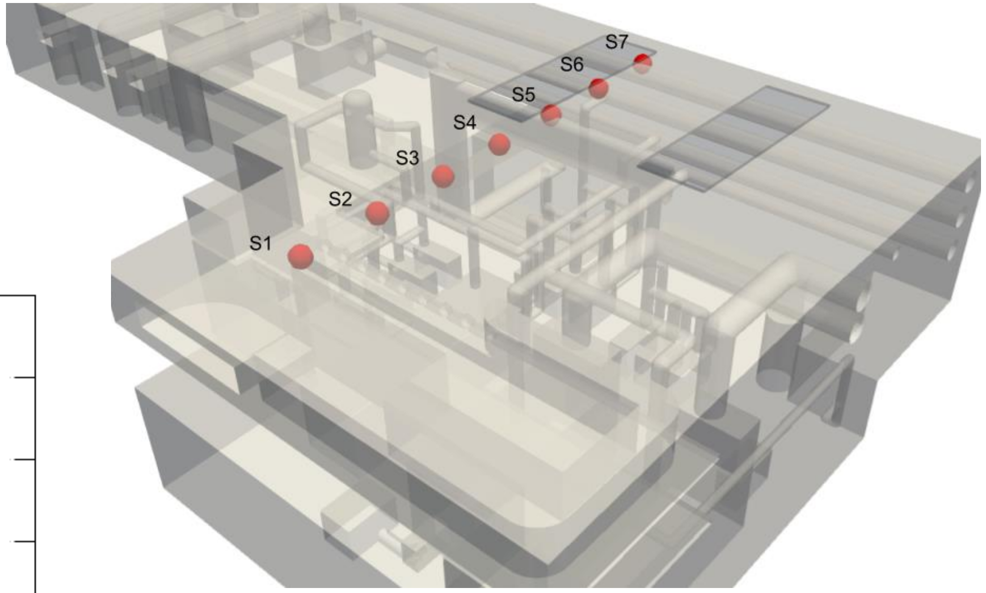




RESULTS

Mechanical vs No ventilation - cloud development

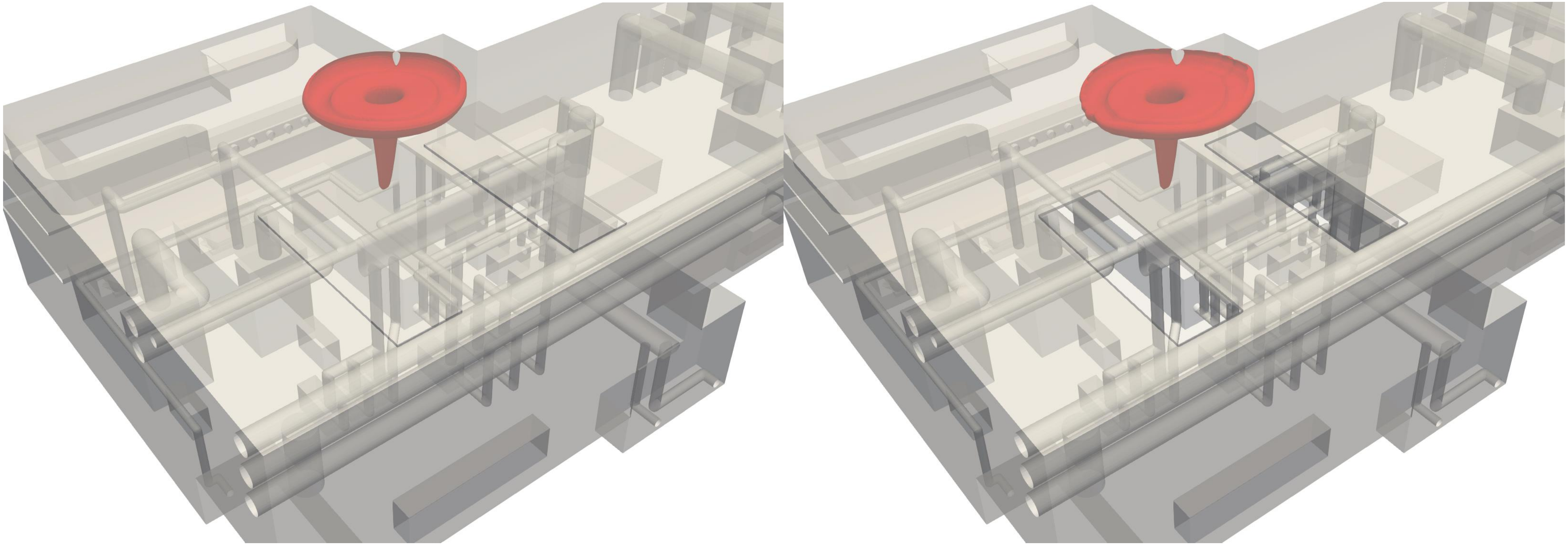




RESULTS

Mechanical vs Natural Ventilation - cloud development (contour surface represents the LFL surface 4%)

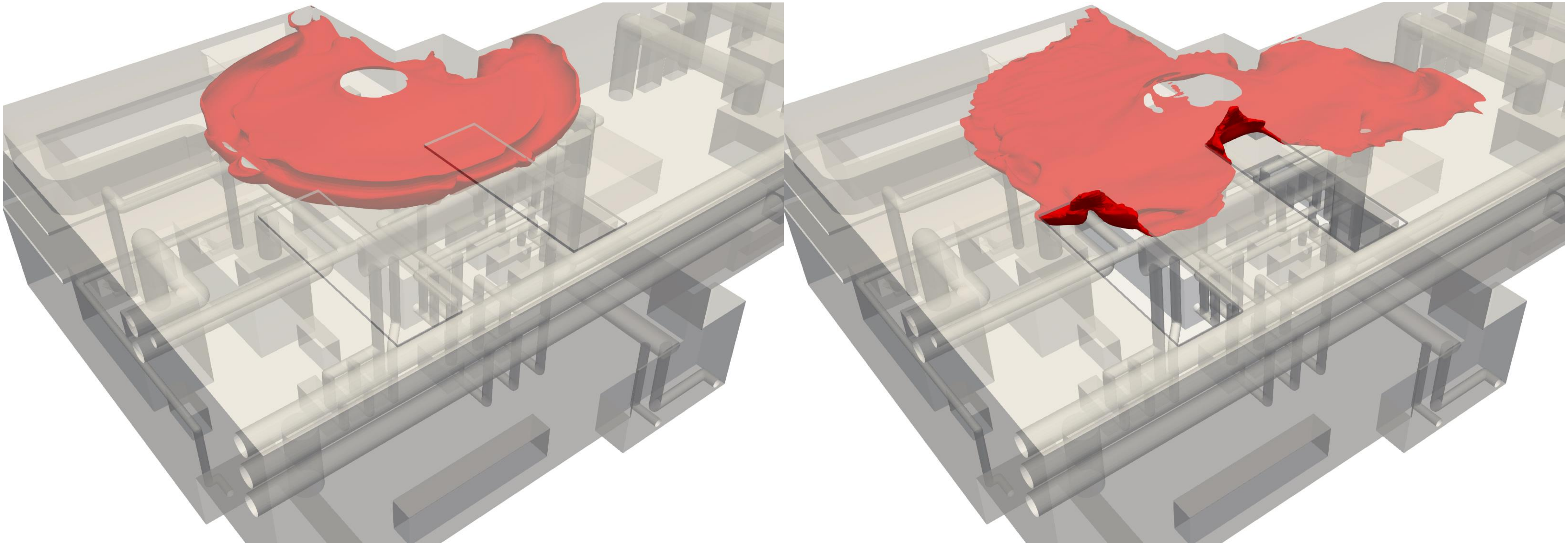
After 5 s



RESULTS

Mechanical vs Natural Ventilation

After 15 s



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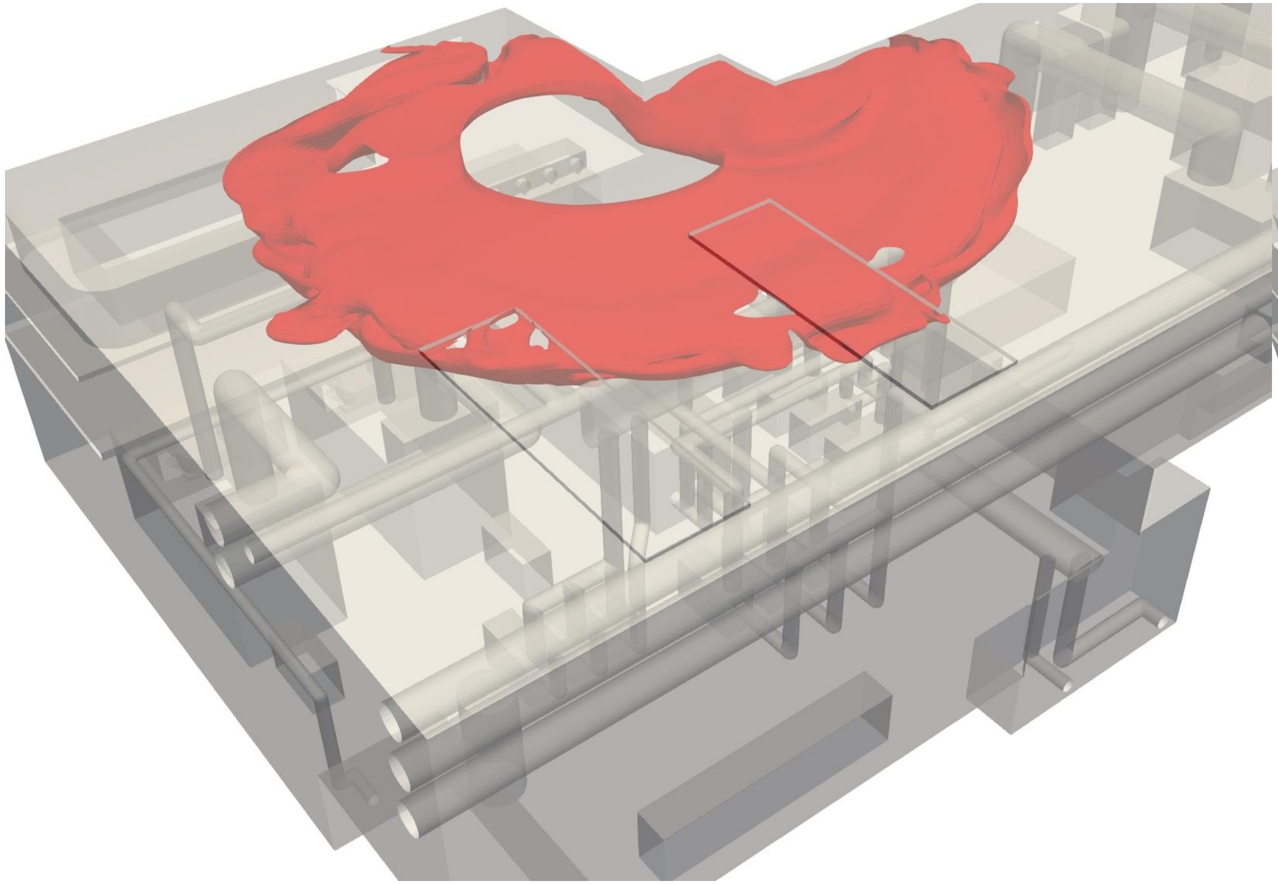
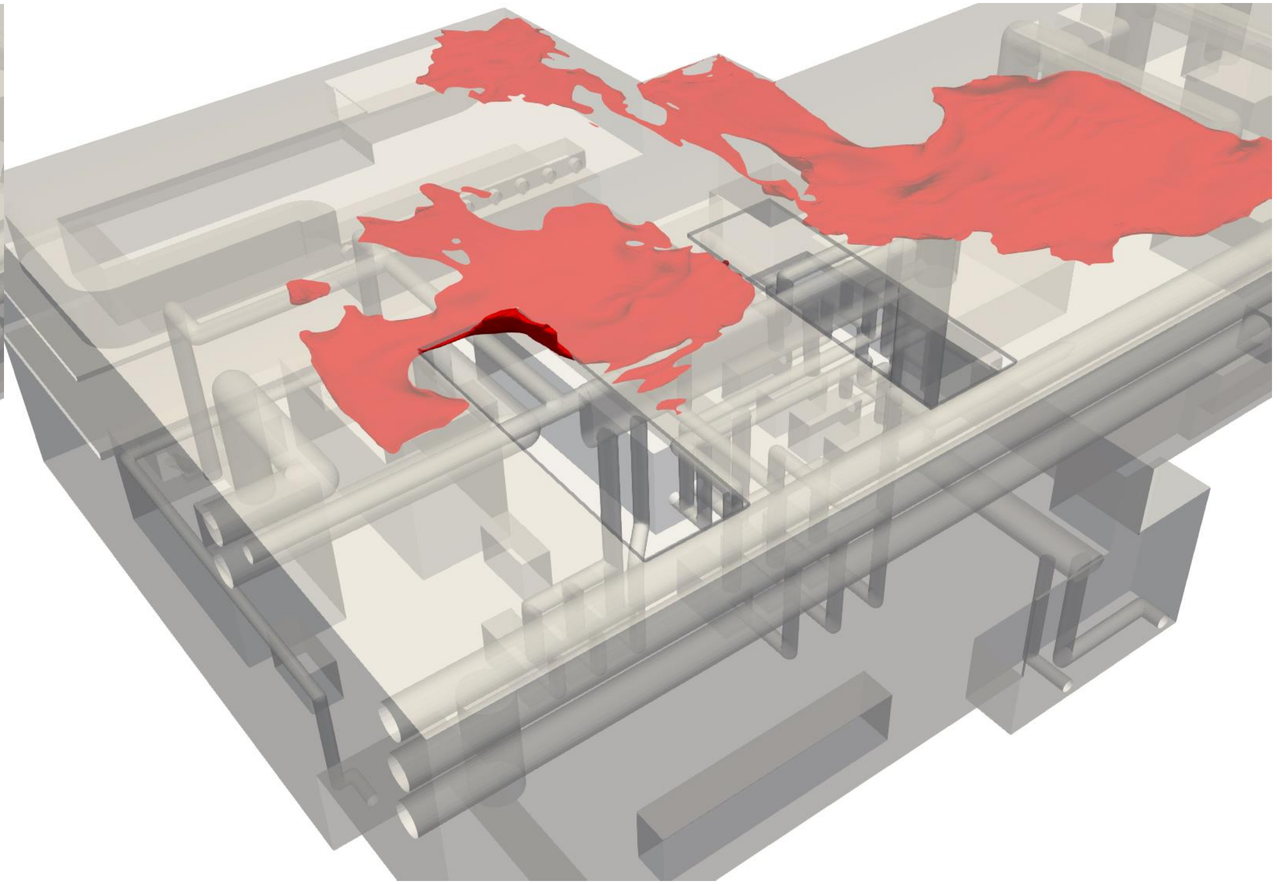
RESULTS

Mechanical vs Natural Ventilation

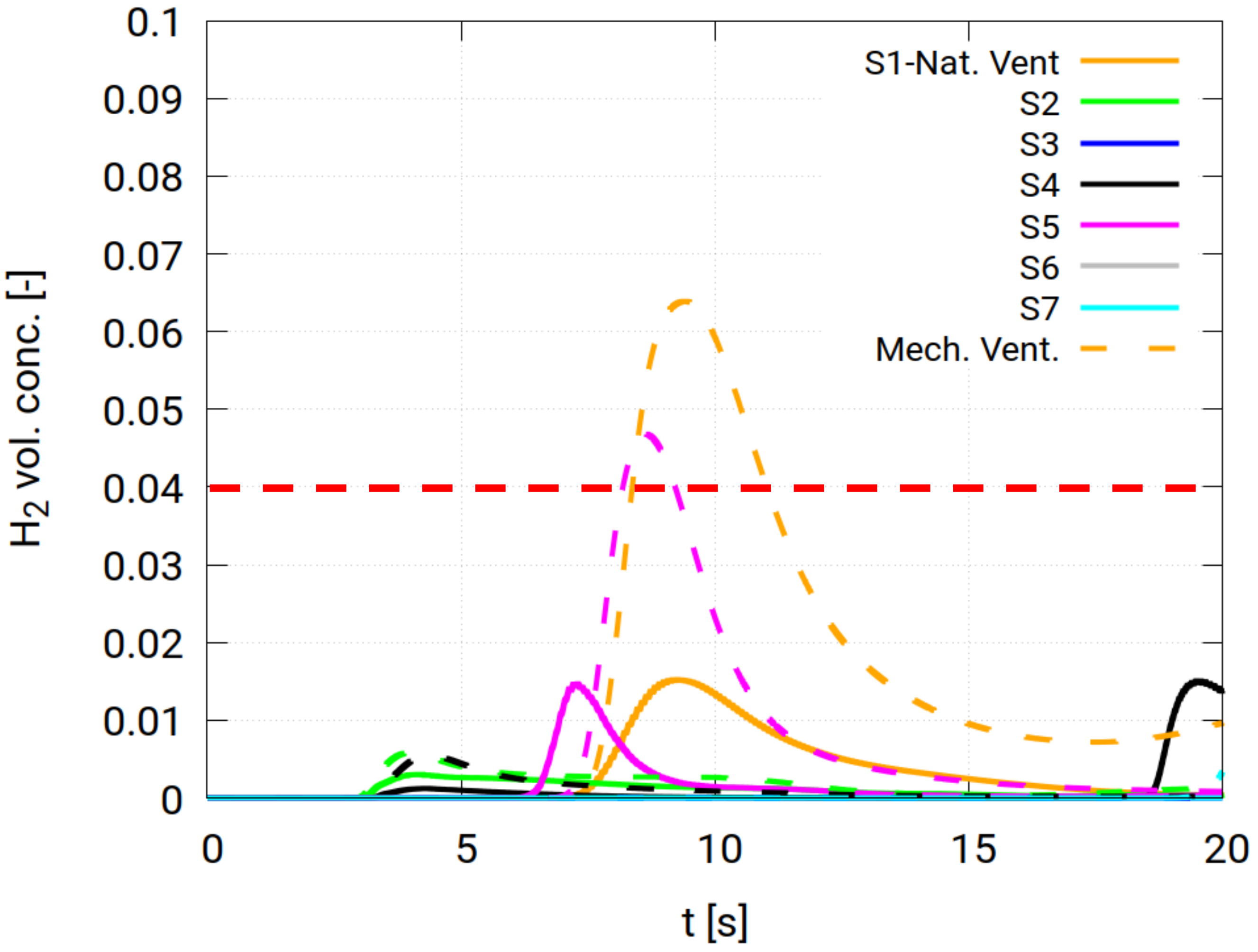
After 20 s

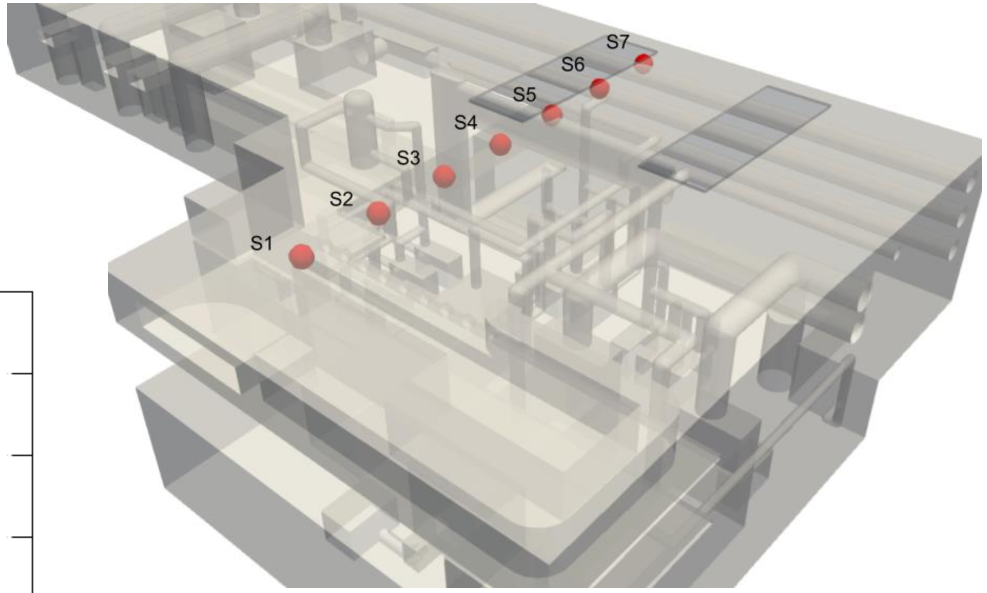




RESULTS

Mechanical vs Natural ventilation - cloud development





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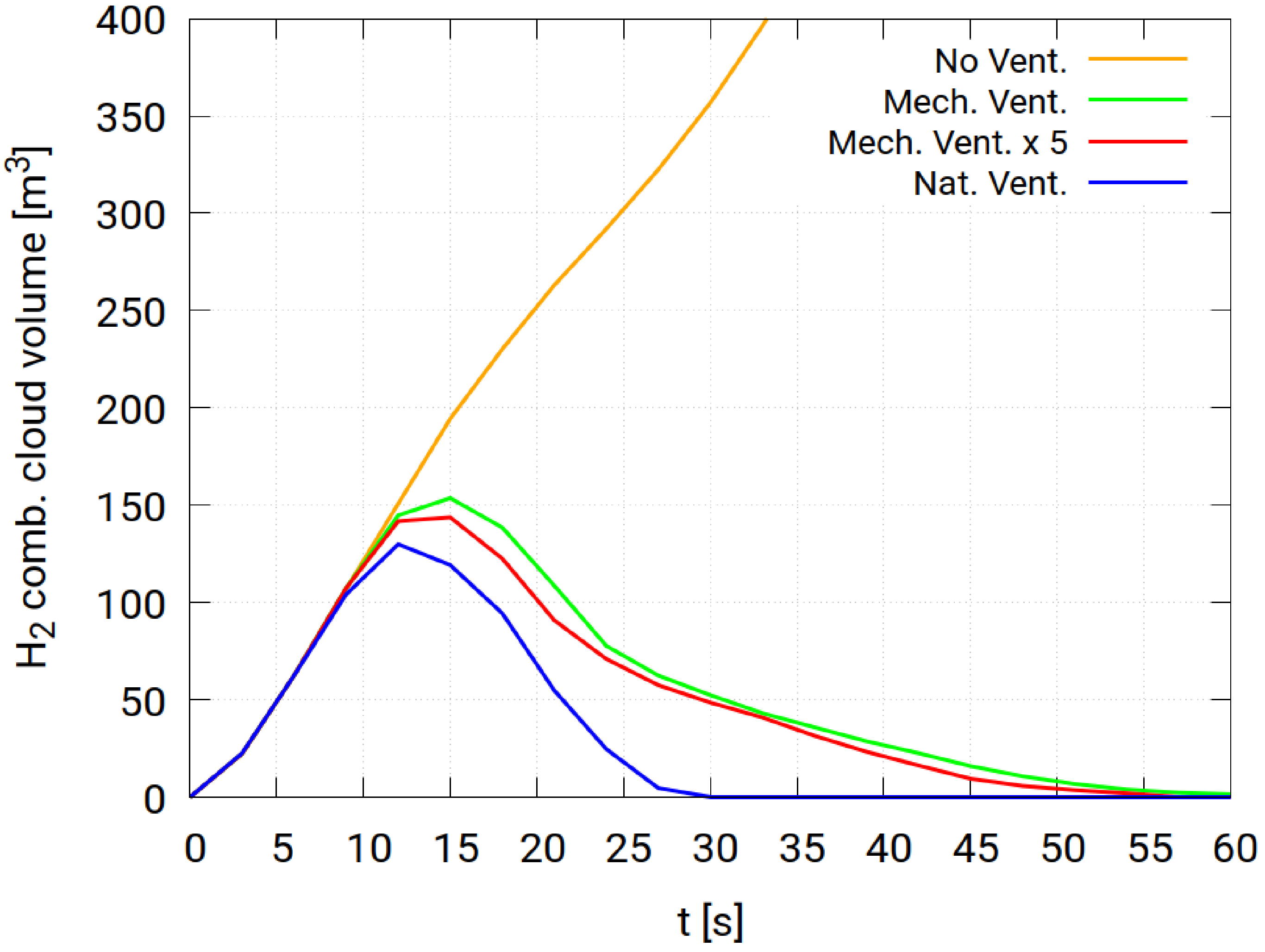
RESULTS

Volume of combustible cloud (i.e. H_2 = 4%-75% vol.)



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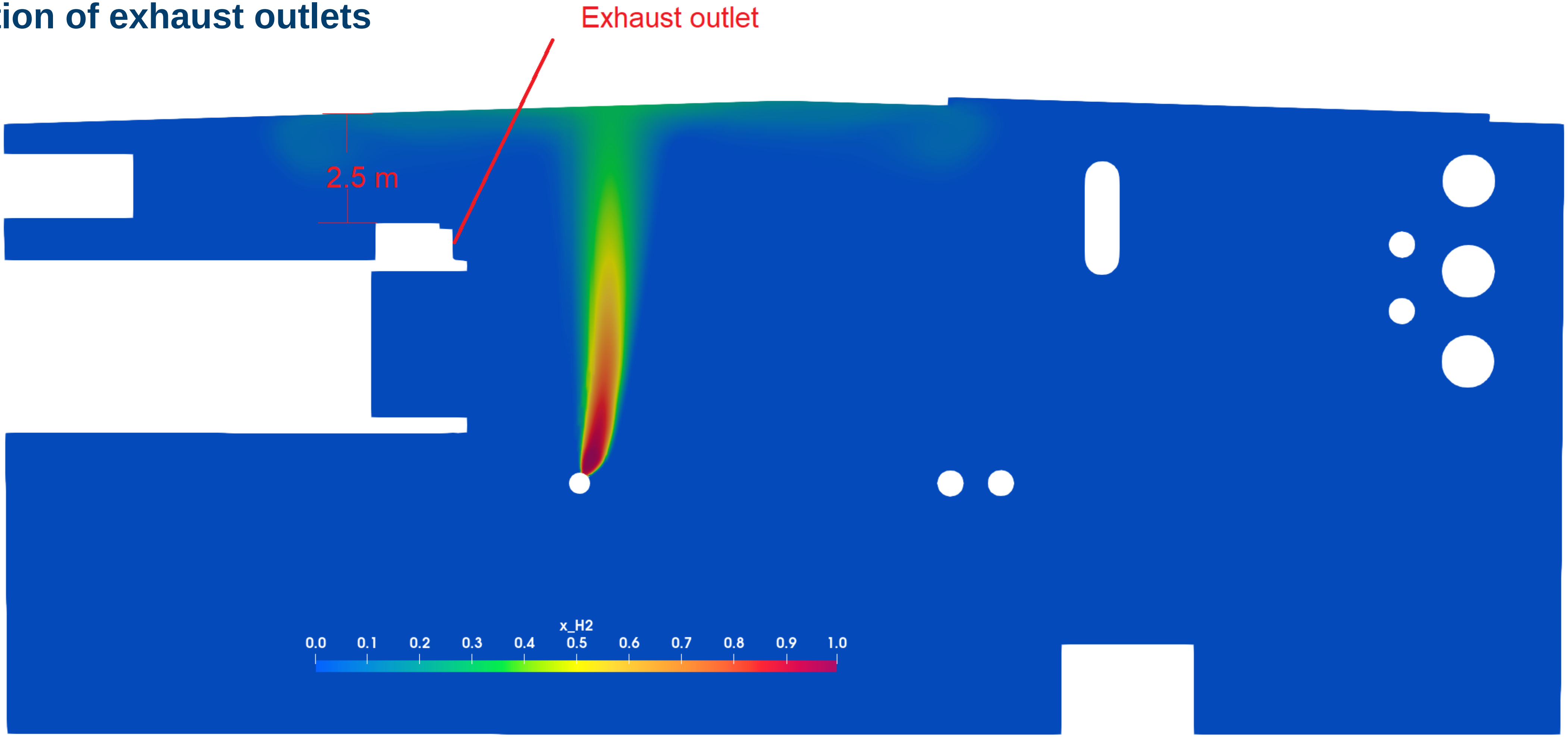
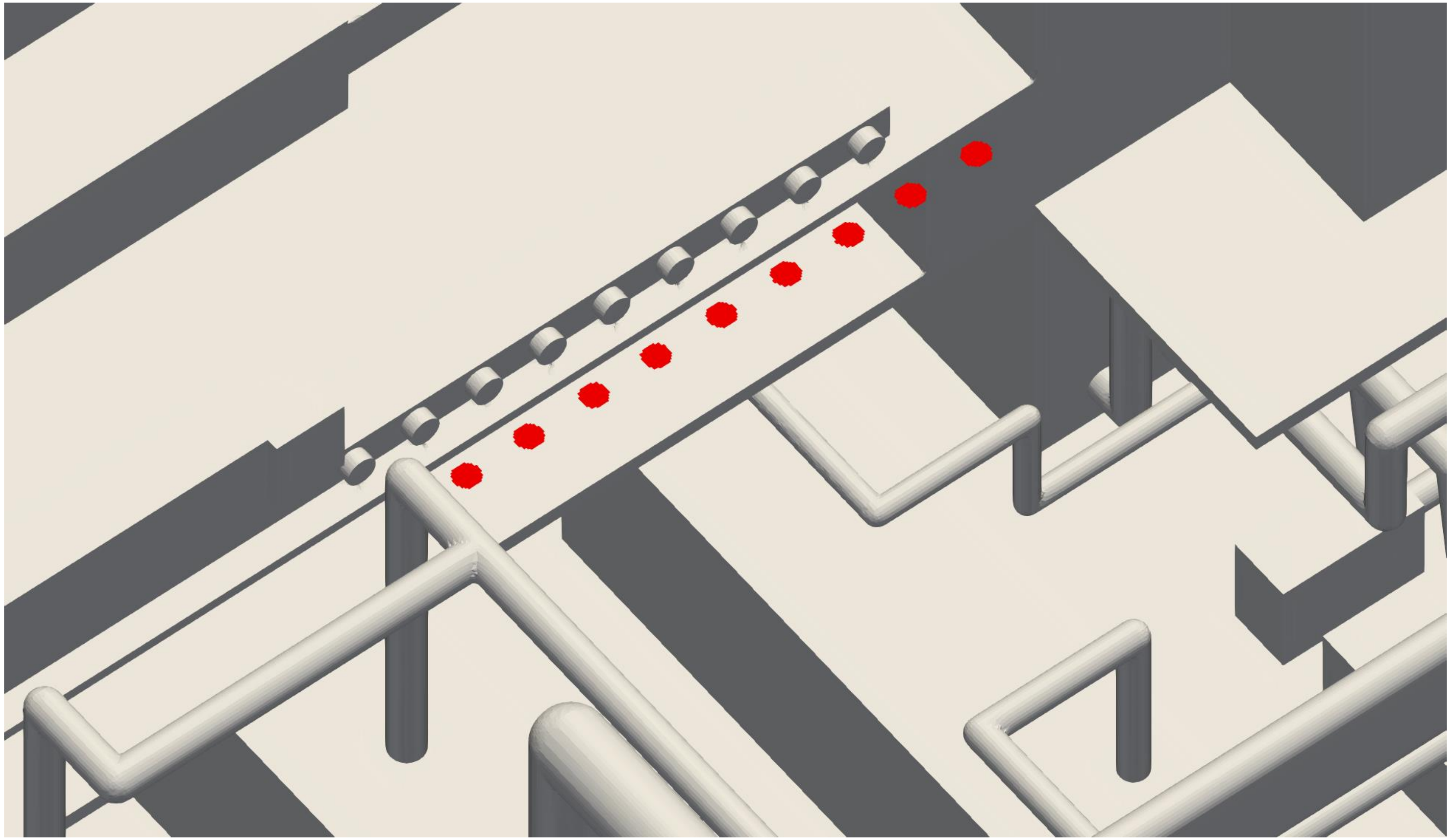
RESULTS

Location of exhaust outlets



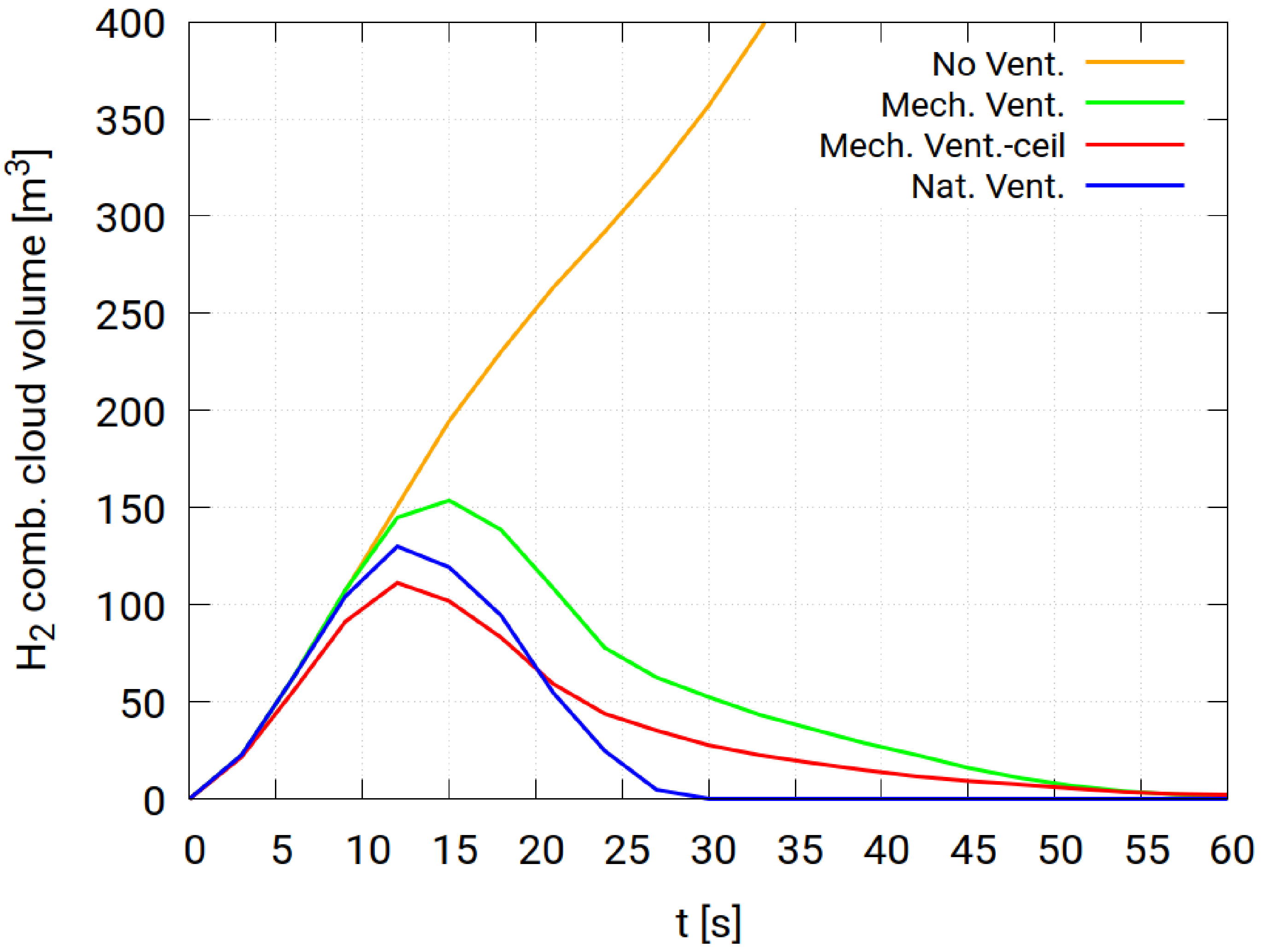
RESULTS

New proposed locations for exhaust outlets



RESULTS

Volume of combustible cloud with the new proposed locations



CONCLUSIONS

The main player in hydrogen cloud dispersion is the buoyancy force

- Natural ventilation from the ceiling is (usually) the most effective
- Exhaust outlets should be in the ceiling or as close as possible to it
- There should be no obstacles between potential hydrogen leakage source and the ceiling
- Overhead structures (ex.: Pipes) tend to break up the cloud which enhances mixing with the air, which increases the cloud volume
- Hydrogen tend to accumulate near the corners between walls and the ceiling
- More studies should be done to study the proper mechanical ventilation rates

FUTURE WORK

- Effects of different leakage locations and directions
- Optimizing sensors’ locations
- Studying the usage of catalytic passive autocatalytic Recombiners (PARs) to mitigate hydrogen accumulation and dispersion in the building

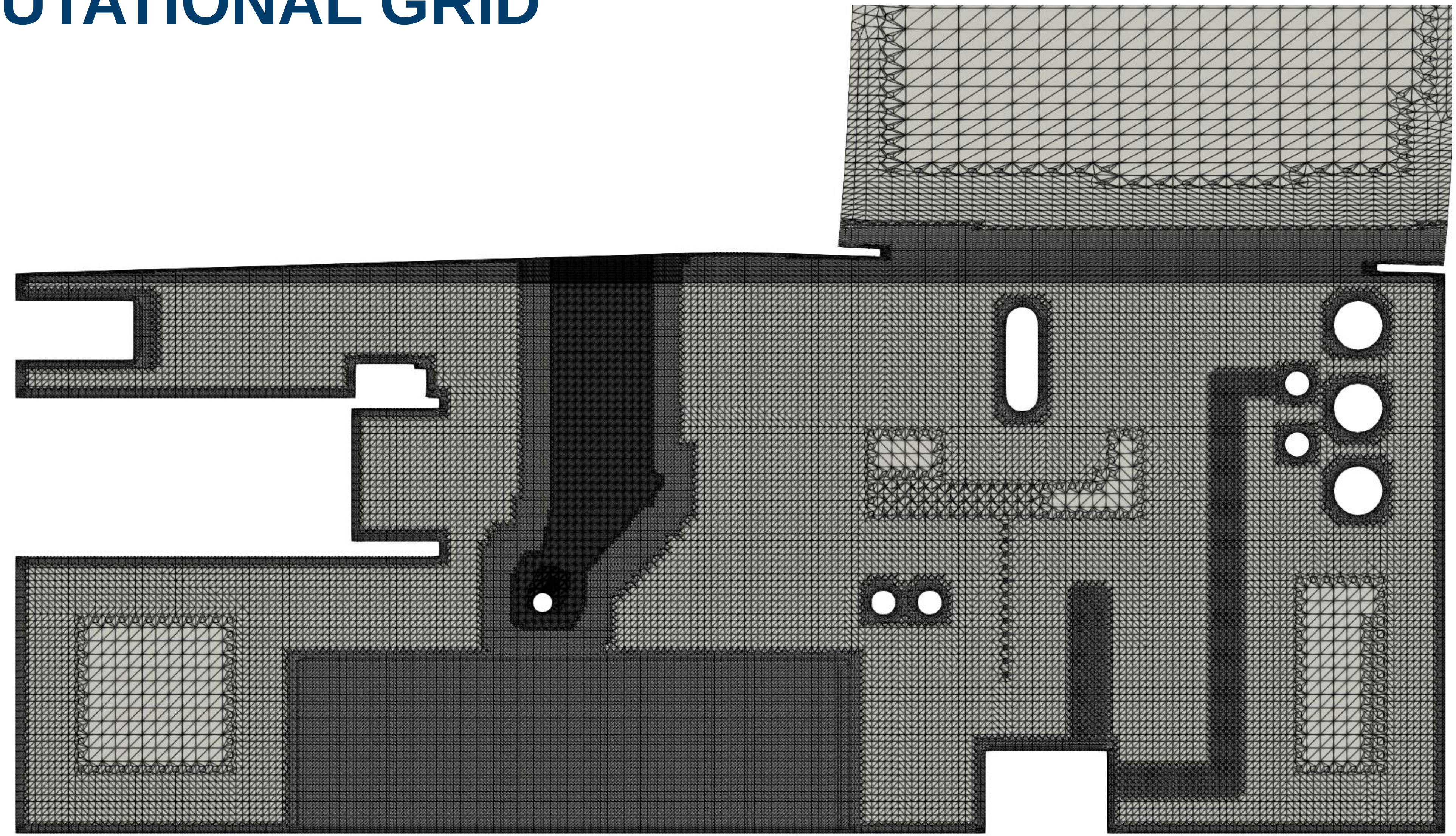
- The Living Lab Energy Campus (LLEC) Power to Gas (PtG++) project is funded by the German Federal Ministry of Education and Research (BMBF) project No.:03SF0573.
- Simulations were carried out using Jülich Super Computer (JSC) for the project grant No. 26701

Contact: k.yassin@fz-juelich.de

Thank you for your attention ! !

Questions?

COMPUTATIONAL GRID



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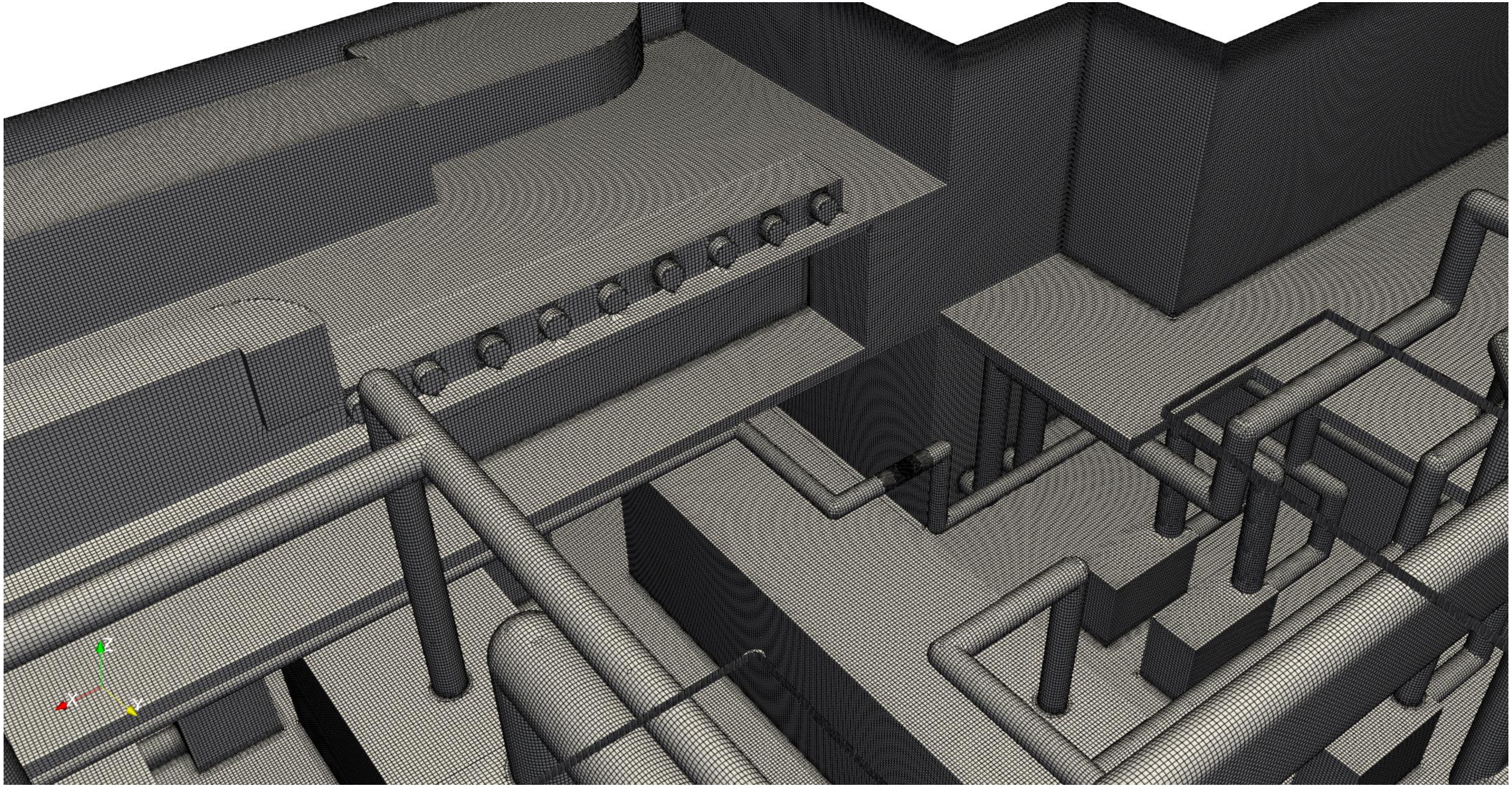
COMPUTATIONAL GRID



INITIAL AND BOUNDARY CONDITIONS

Variable	External walls		Internal walls		Air inlet		Atmosphere		Exhaust outlets		Domain Iinit.
	BC	Init.	BC	Init.	BC	Init.	BC	Init.	BC	Init.	
p	fixedFluxPresure	1 bar	fixedFluxPresure	1 bar	inletOutlet	1 bar	inletOutlet	1 bar	fixedFluxPresure	1 bar	1 bar
T	zeroGradient	-	zeroGradient	-	inletOutlet	298.15 K	inletOutlet	298.15 K	zeroGradient	-	298.15 K
U	No slip	(0,0,0)	No slip	(0,0,0)	inletOutlet	(0,0,0)	inletOutlet	(0,0,0)	Flow Rate Velocity	0.48567, 1.543 m3/s	
nut	SpaldingWall Function	1.00E-07	SpaldingWall Function	1.00E-07	inletOutlet	1.00E-07	inletOutlet	1.00E-07	calculated	1.00E-07	1.00E-07
k	kqR Wall Function	1.35E-05	kqR Wall Function	1.35E-05	inletOutlet	1.35E-05	inletOutlet	1.35E-05	zeroGradient	1.35E-05	1.35E-05
ω	omega Wall Function	1.00E-07	omega Wall Function	1.00E-07	inletOutlet	1.00E-07	inletOutlet	1.00E-07	zeroGradient	1.00E-07	1.00E-07
H_2	zeroGradient	-	zeroGradient	-	inletOutlet	0	inletOutlet	0	zeroGradient	-	0
O_2	zeroGradient	-	zeroGradient	-	inletOutlet	0.2328	inletOutlet	0.2328	zeroGradient	-	0.2328
N_2	zeroGradient	-	zeroGradient	-	inletOutlet	0.7672	inletOutlet	0.7672	zeroGradient	-	0.7672

NUMERICAL SOLVERS, SCHEMES, AND CONVERGENCE CRITERIA

Variable	Solution		div. Scheme
	Solver	tol.	
p	GAMG	1.00E-06	Gauss upwind
T	PBiCGStab	1.00E-06	Gauss upwind
U	PBiCGStab	1.00E-06	Gauss linearUpwind grad(U)
nut	PBiCGStab	1.00E-06	Gauss linear
k	PBiCGStab	1.00E-06	Gauss upwind
ω	PBiCGStab	1.00E-06	Gauss upwind
H_2	PBiCGStab	1.00E-06	Gauss upwind
O_2	PBiCGStab	1.00E-06	Gauss upwind
N_2	PBiCGStab	1.00E-06	Gauss upwind

Time	Euler
Grad.	cellMDLimited Gauss linear 0.5
Laplacian	Gauss linear limited 0.5
Interpol.	linear

TURBULENCE MODEL

k-ω SST with Simple Gradient Diffusion Hypothesis (SGDH)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{U}\right) = 0$$

$$\frac{\partial \rho \vec{U}}{\partial t} + \nabla \cdot \left(\rho \vec{U} \otimes \vec{U}\right) = -\nabla p + \nabla \cdot \tau + \rho \vec{g}$$

$$\frac{\partial \rho h_{tot}}{\partial t} + \nabla \cdot \left(\rho \vec{U} h_{tot}\right) = \frac{\partial p}{\partial t} - \nabla \cdot \dot{\vec{q}}'' + \nabla \cdot (\vec{U} \cdot \tau) + \vec{U} \cdot (\rho \vec{g}) - \nabla \cdot \dot{\vec{q}}''_{rad}$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \left(\rho \vec{U} Y_i\right) = -\nabla \cdot \vec{J}_i$$

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TURBULENCE MODEL

k-ω SST with Simple Gradient Diffusion Hypothesis (SGDH)

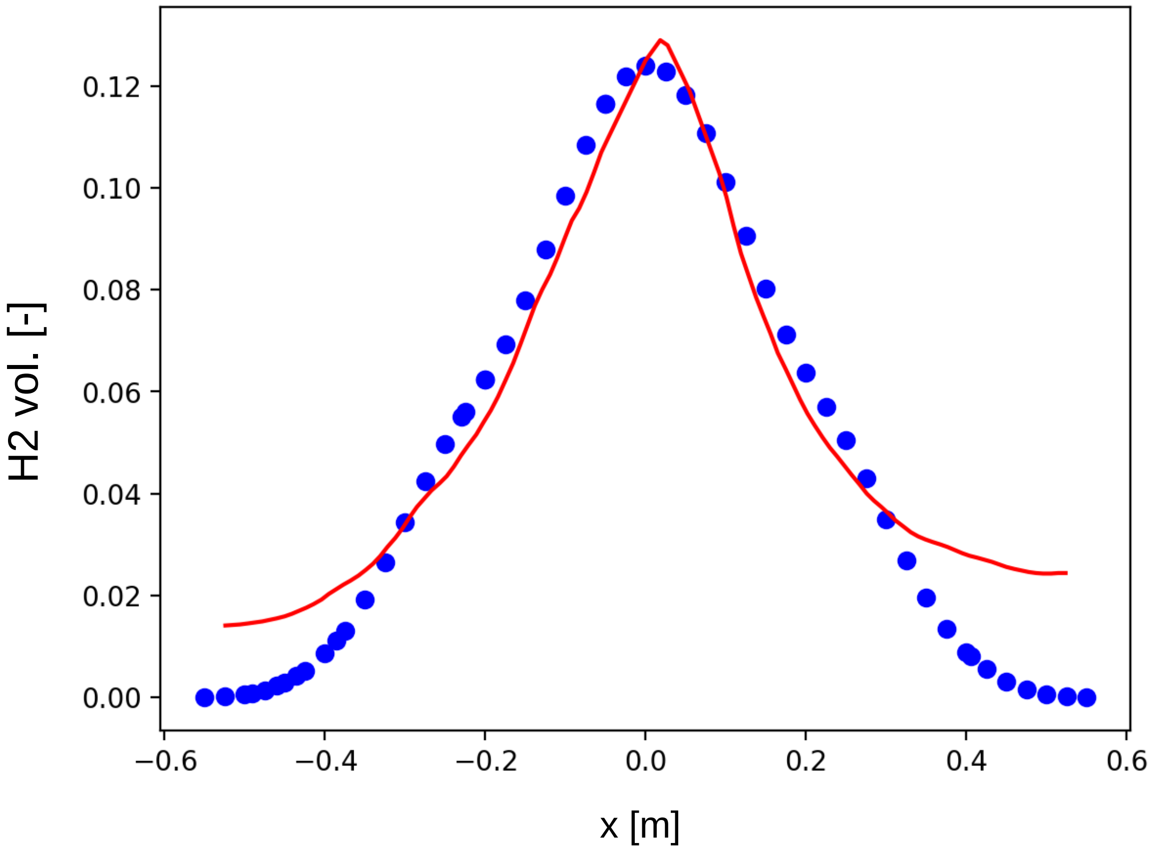
$$\frac{\partial\left(\rho k\right)}{\partial t} + \nabla\cdot(\rho\vec{U}k) = \nabla\cdot\Big(\big(\mu+\mu_t\sigma_k\big)\nabla k\Big) + \tilde{P}_k - \rho\beta^*\omega k + P_{k,b}$$

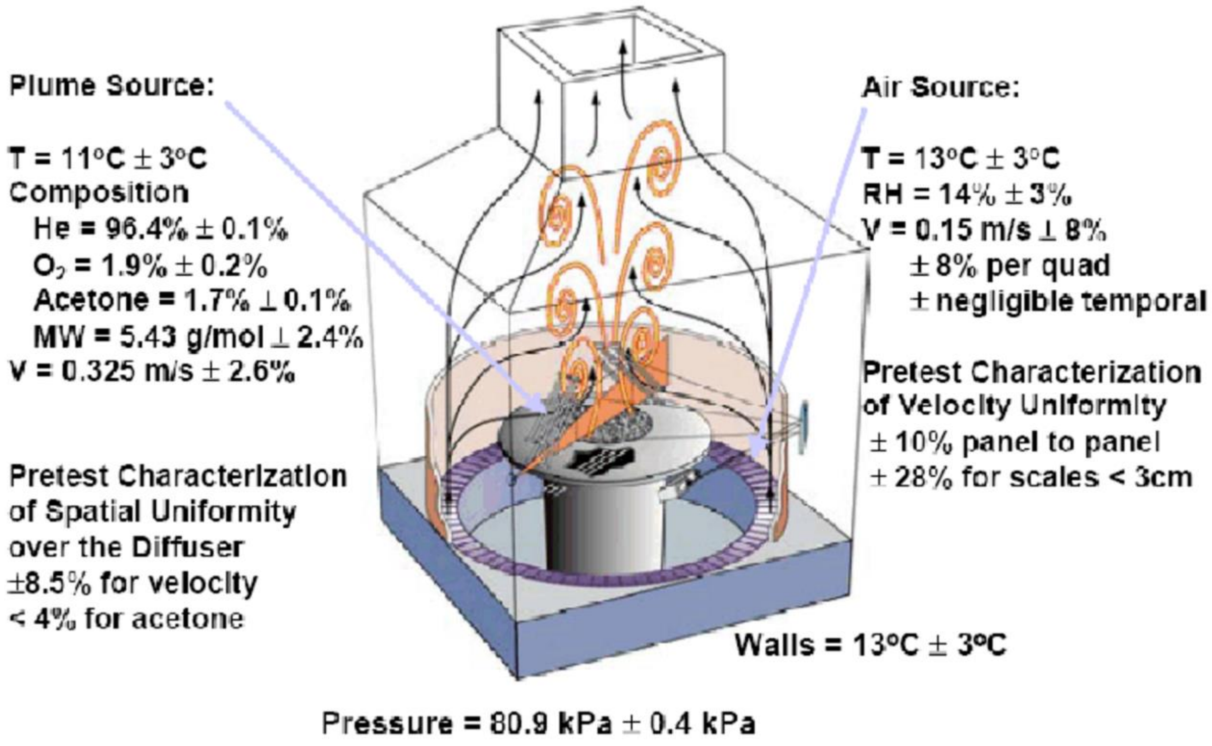
$$\frac{\partial\left(\rho\omega\right)}{\partial t} + \nabla\cdot(\rho\vec{U}\omega) = \nabla\cdot\Big(\big(\mu+\mu_t\sigma_\omega\big)\nabla\omega\Big) + 2\left(1-F_1\right)\frac{\rho\sigma_{\omega 2}}{\omega}\nabla k\cdot\nabla\omega + P_\omega + P_{\omega,b} - Y_\omega$$

$$P_{\omega,b} = \nu_t((\gamma+1)C_3\cdot max(P_{k,b},0) - P_{k,b})$$

$$P_{k,b} = -\frac{\nu_t}{\sigma_\rho}g_i\frac{\partial\rho}{\partial x_i}$$

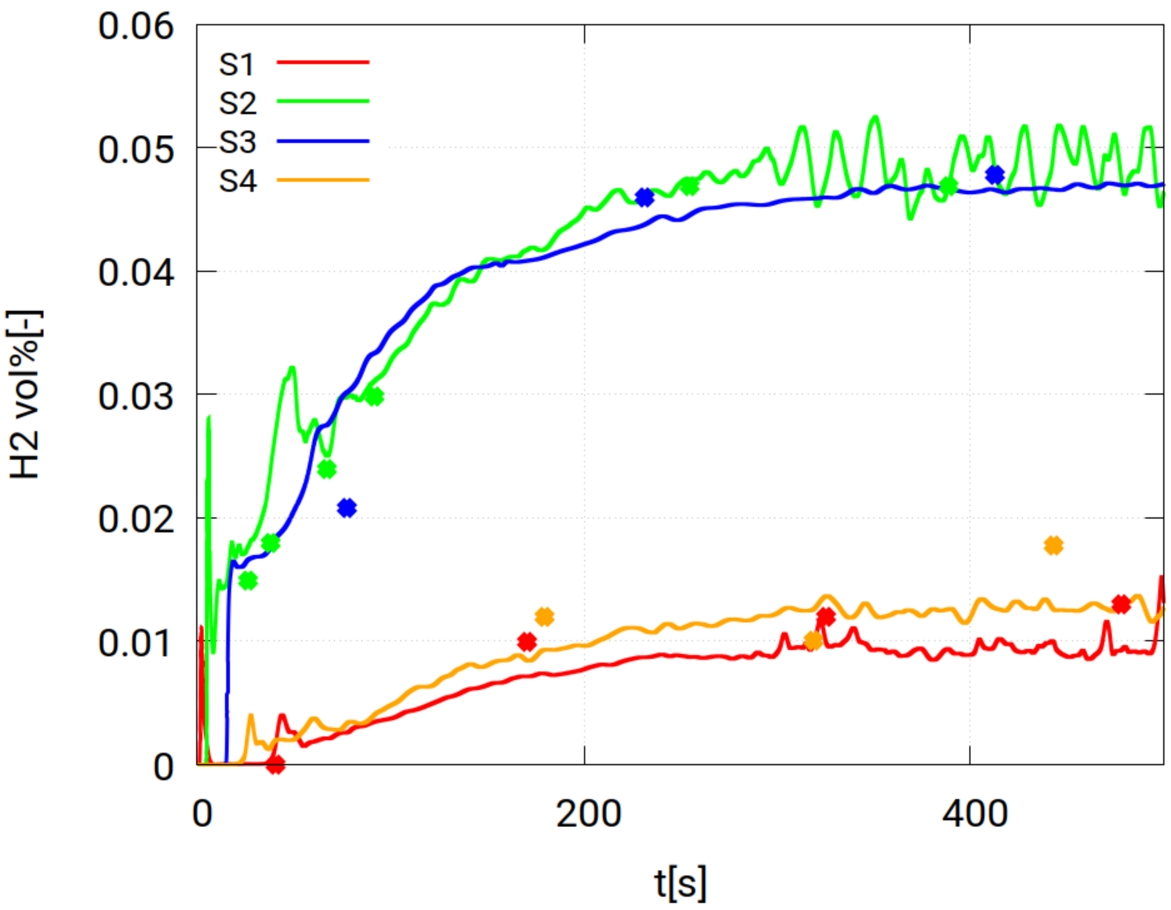
VALIDATION AND VERIFICATION: FLAME EXP.

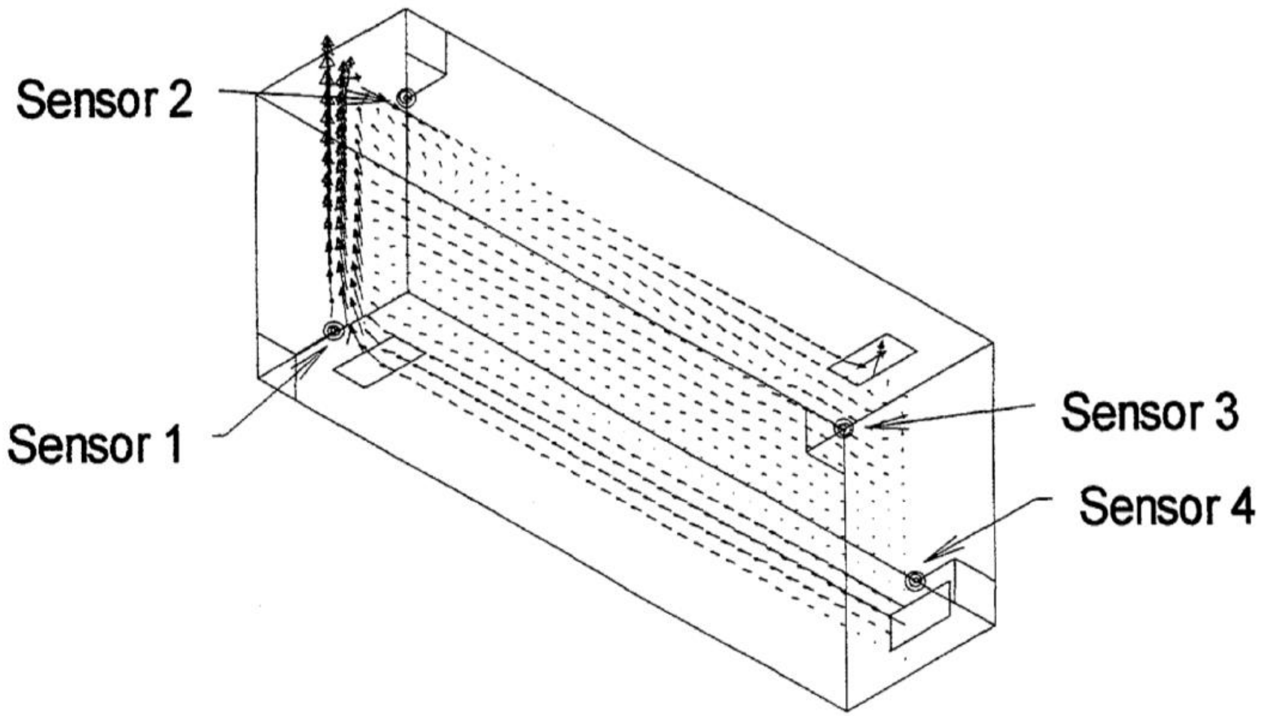




O'hern, T. J., Weckman, E. J., Gerhart, A. L., Tieszen, S. R., & Schefer, R. (2005). Experimental study of a turbulent buoyant helium plume. *Journal of Fluid Mechanics*, *544*, 143-171.

VALIDATION AND VERIFICATION: FLAME EXP.

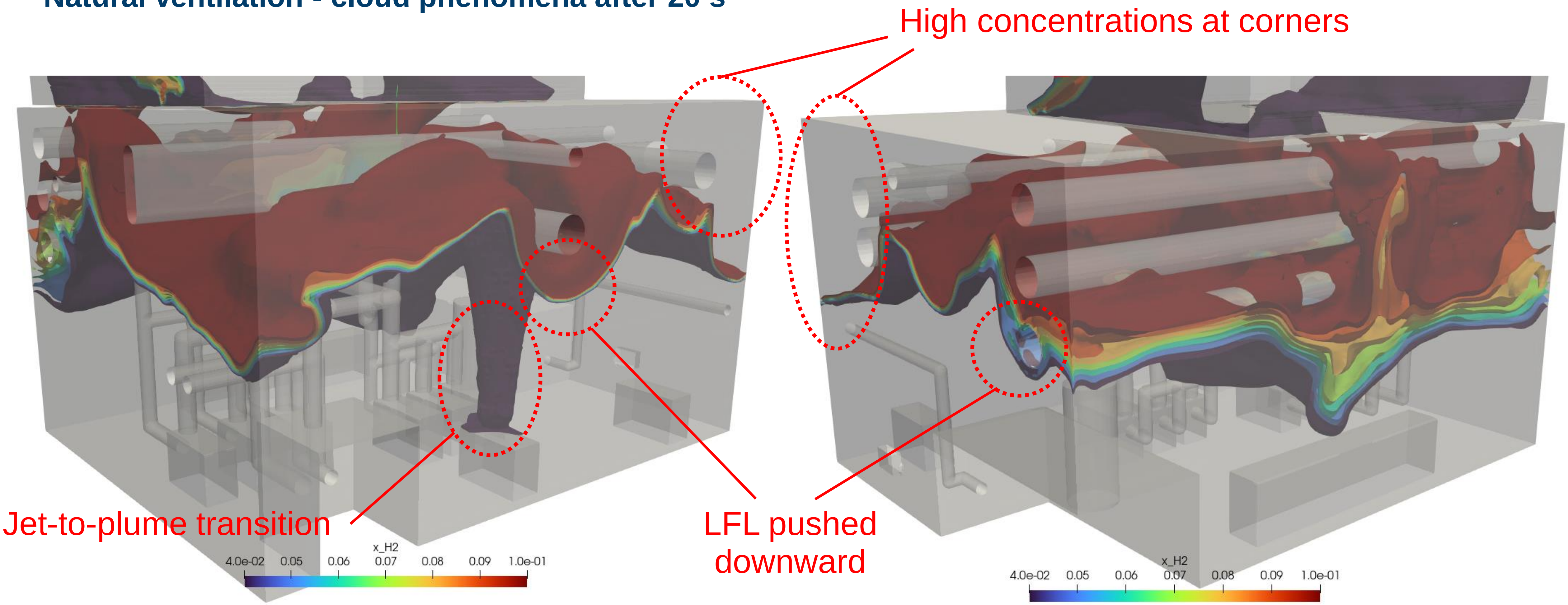




Swain, M. R., Grilliot, E. S., & Swain, M. N. (1998). *Risks incurred by hydrogen escaping from containers and conduits* (No. NREL/CP-570-25315-Vol. 2; CONF-980440-Vol. 2). National Renewable Energy Lab.(NREL), Golden, CO (United States).

RESULTS

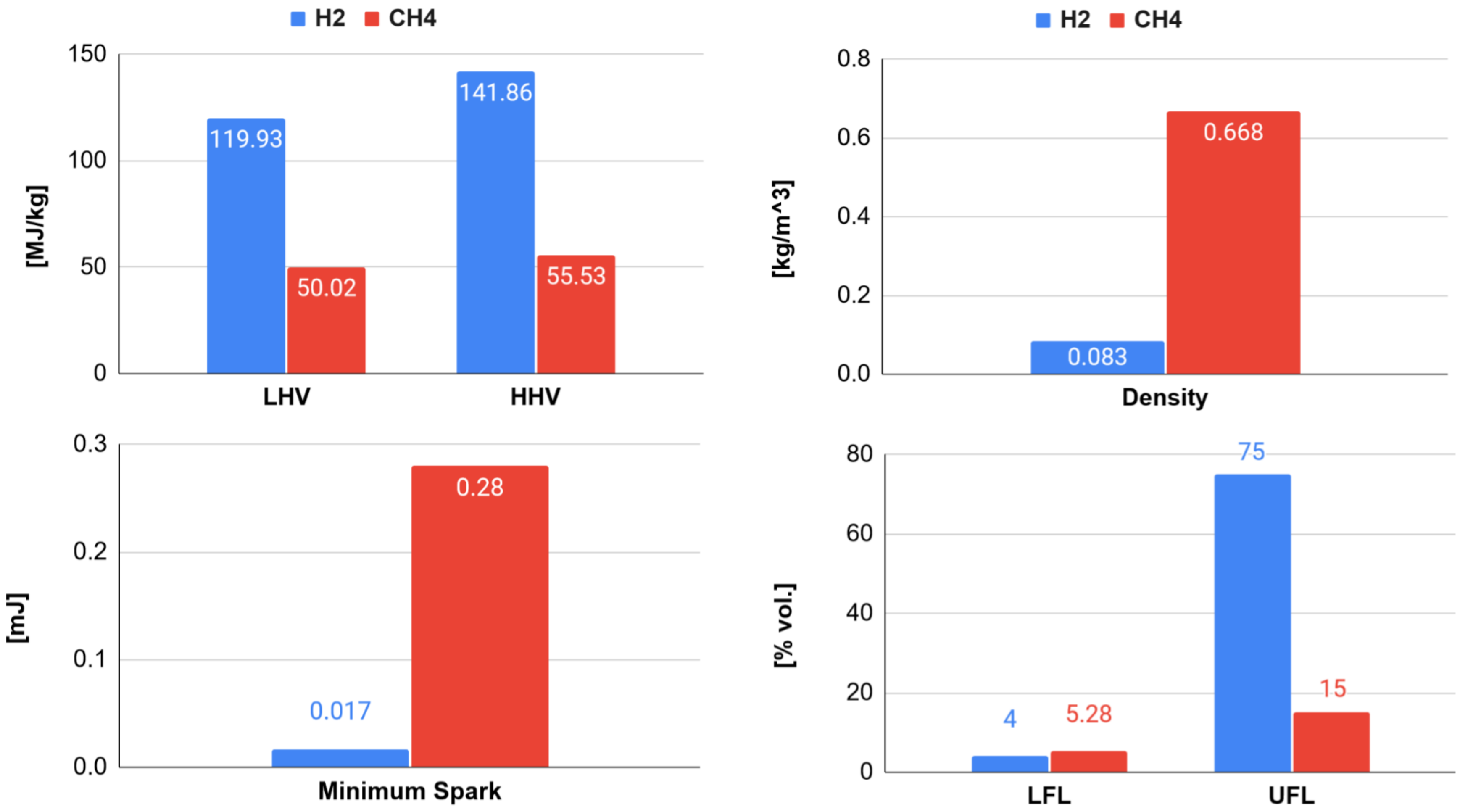
Natural ventilation - cloud phenomena after 20 s



Iso-surfaces after 20 s

MOTIVATION

But…hydrogen has extreme physical properties



📖 Kotchourko, A. and Jordan, T. eds., 2022. *Hydrogen Safety for Energy Applications: Engineering Design, Risk Assessment, and Codes and Standards*. Butterworth-Heinemann.

METHODOLOGY

Phenomena occurring during GH2 leakage

GH_2 leakage simulation

Diffusion: Between different gases (H_2 and air) during the leakage

Turbulent jet: At the leakage point due to high pressure in the piping system

Buoyancy: Stratification, cloud formation near the ceiling, and natural ventilation through roof openings

H2 Cloud distribution: Risk of ignition if concentration exceeds LFL (4% vol.)

THE LIVING LAB ENERGY CAMPUS (LLEC) AT FZ JÜLICH

Scope of work

Identify the different leakage scenarios in the building: Locations, ventilation, response time…etc

Calculate leakage parameters for each case: Leakage flow rate, temperature, duration

Simulate cloud dispersion inside the building for free and forced ventilation at different rates

Analyze the hydrogen cloud development

Optimal locations of the sensors for each system

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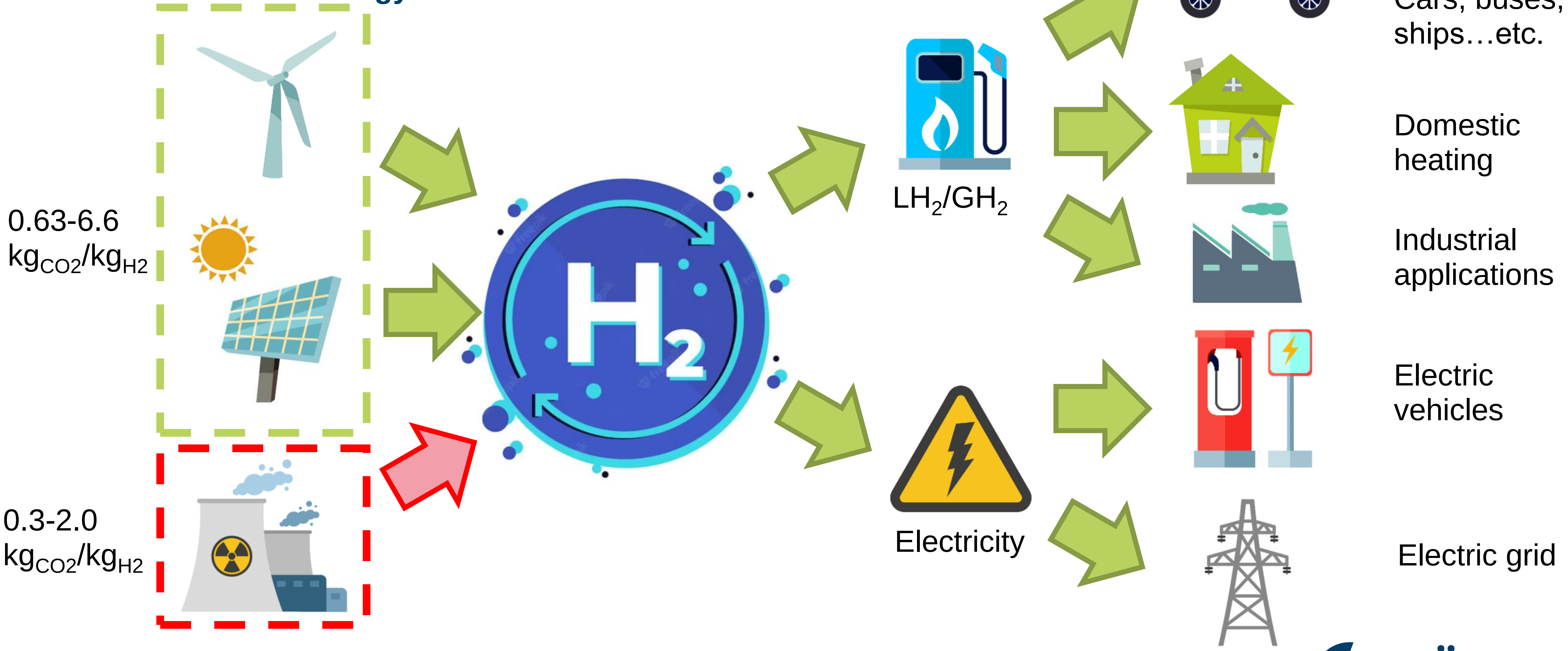
MOTIVATION

A corner stone for energy transition



📖 Aziz M. Liquid hydrogen: A review on liquefaction, storage, transportation, and safety. Energies. 2021 Sep 17;14(18):5917.

Remove the first motivation slide

Say more about the building and its complixty

We are transferring experience from Nuclear applications to Hydrogen applications