

ΗΜΕΡΙΔΑ ΥΠΟΤΡΟΦΩΝ ΙΠΤΑ
ΔΗΜΟΚΡΙΤΟΣ
28/03/07

«Μοντελοποίηση διασποράς υδρογόνου και άλλων ανωστικών αερίων σε κλειστούς χώρους με τη μεθοδολογία της υπολογιστικής ρευστομηχανικής»

Παπανικολάου Ευθυμία
Χημικός Μηχανικός
Υποψήφια Διδάκτωρ ΕΜΠ
Υπεύθυνος Ερευνητής ΙΠΤΑ: Α. Βενετσάνος
Υπεύθυνος Καθηγητής ΕΜΠ: Ν. Μαρκάτος



OBJECTIVES

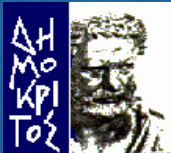
- Evaluation and further development of the ADREA-HF code, with emphasis on hydrogen and other buoyant gas release and dispersion in confined spaces.

Development and implementation of different turbulence models will be one of the main objectives of this work.

- To validate the performance of the new features of the code, the results of the simulations will be compared with results from physical experiments with hydrogen-air and other buoyant gas-air mixtures such as helium.

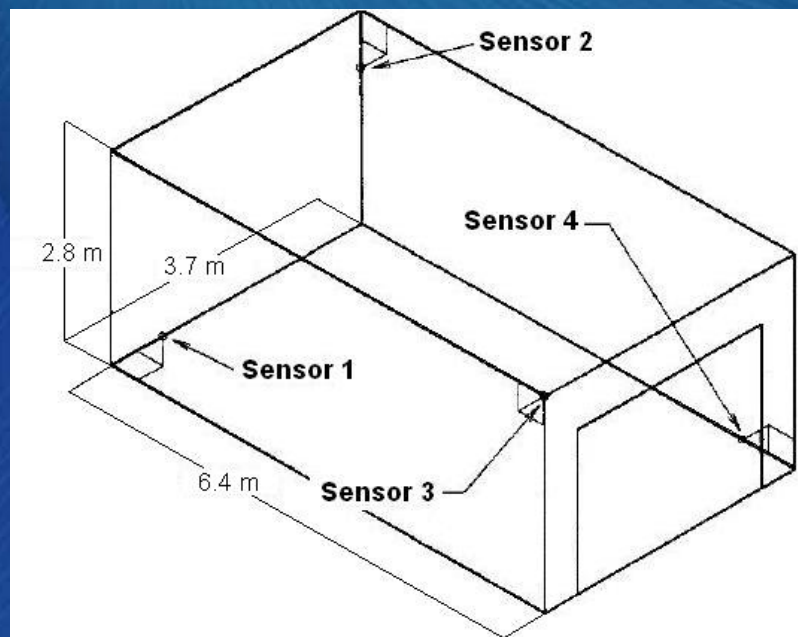
- Investigation of mitigation techniques for minimizing the effects of the leaked gas and possible explosion events.

It is thought that such information can contribute to practice guidelines for confined spaces in terms of safety.

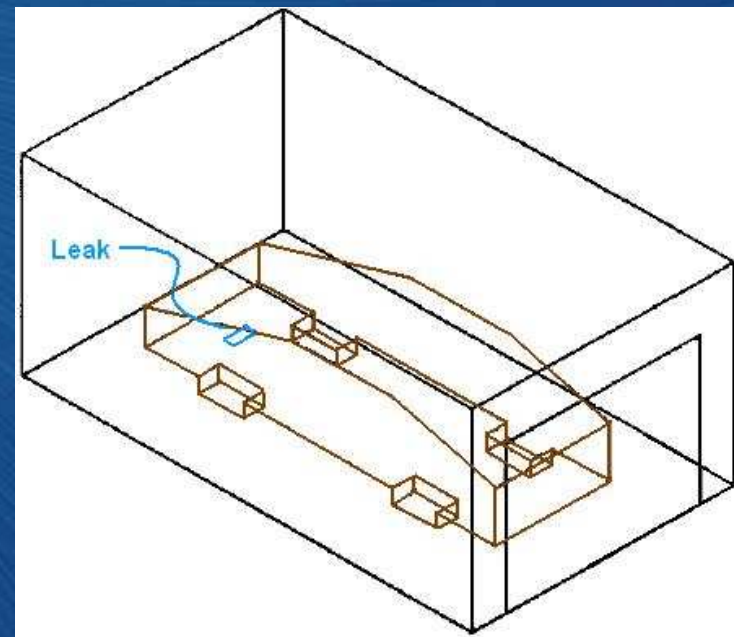


CFD Simulations – Helium release in a private garage (1)
(ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

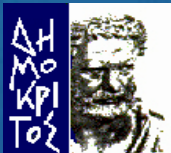
Experimental description (Swain et. al. 1998)



Single car garage facility and
sensors' location

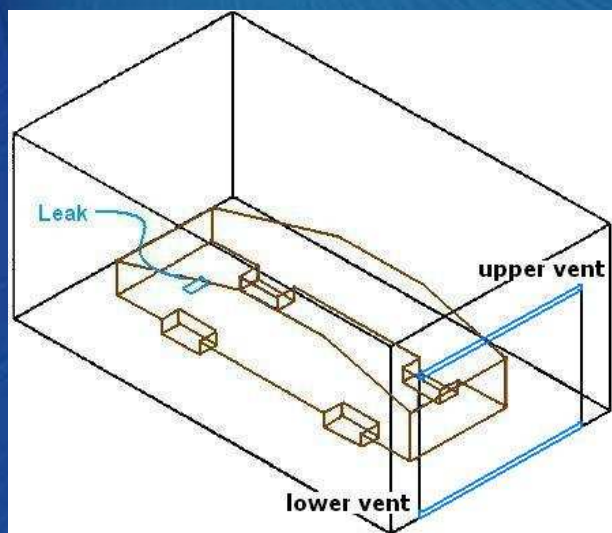


Vehicle and leak location

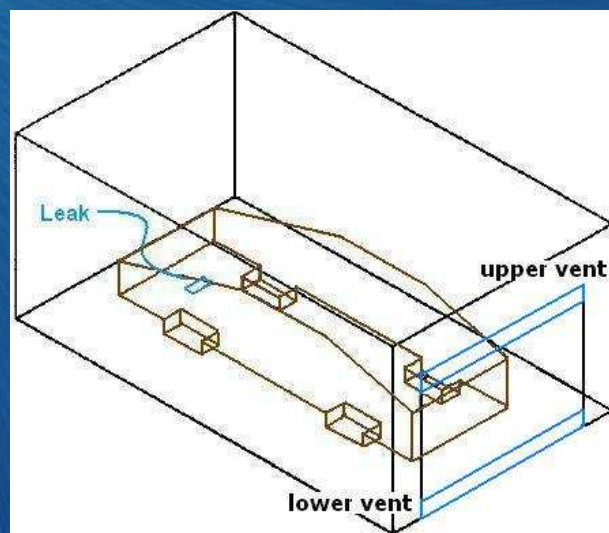


CFD Simulations – Helium release in a private garage (2) (ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

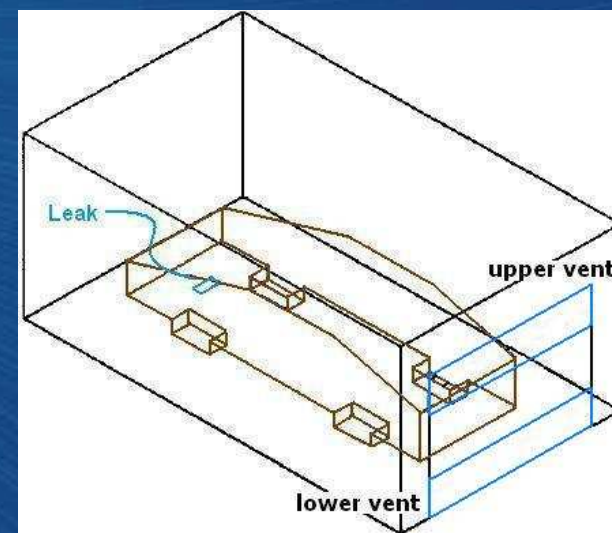
Experimental description (Swain et. al. 1998)



Case 1: 2.5 inches (6.35 cm) top and bottom vents

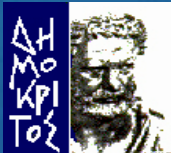


Case 2: 9.5 inches (24.13 cm) top and bottom vents



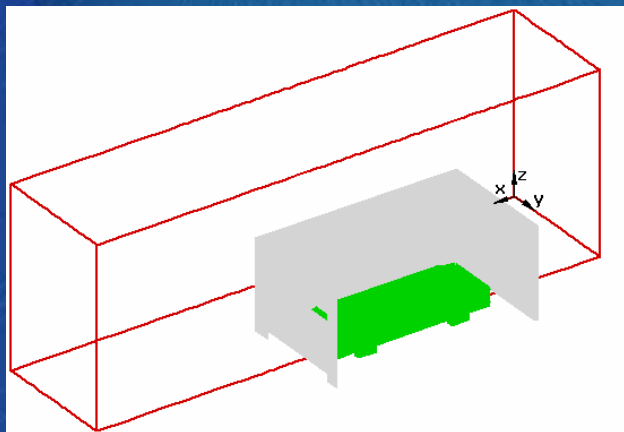
Case 3: 19.5 inches (49.53 cm) top and bottom vents

Leak: 7.200 lt/hr He for 2 hours, directed downwards

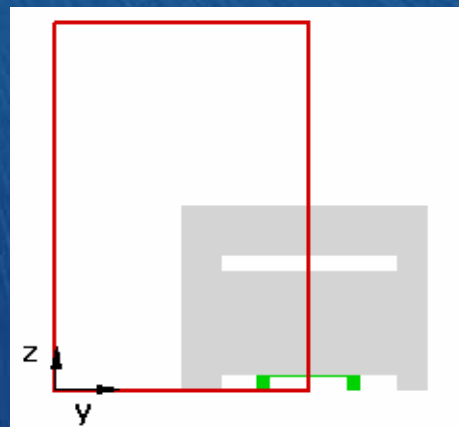


CFD Simulations – Helium release in a private garage (3) (ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

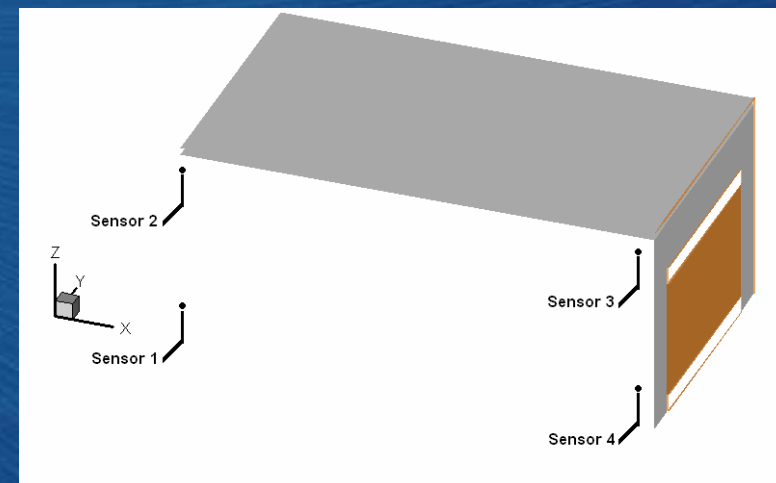
Computational Domain



Domain extends beyond
garage's boundary



x-z plane symmetry assumption
given leak location and facility's
geometry



Sensors located on the same side
given symmetry assumption

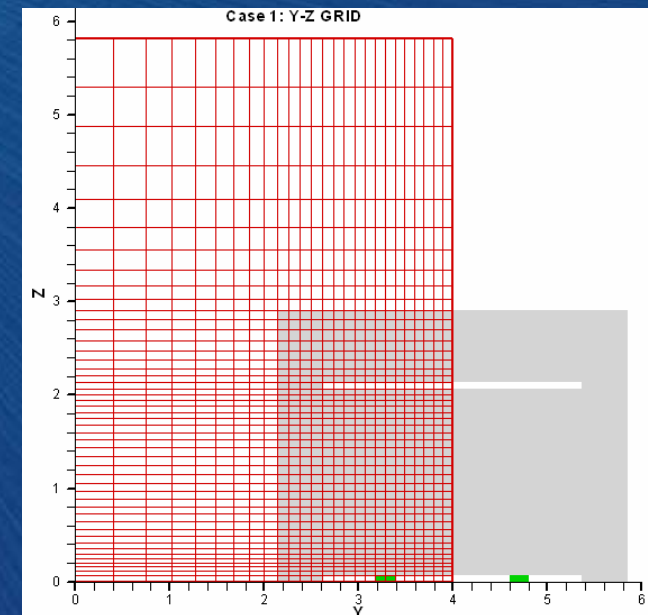
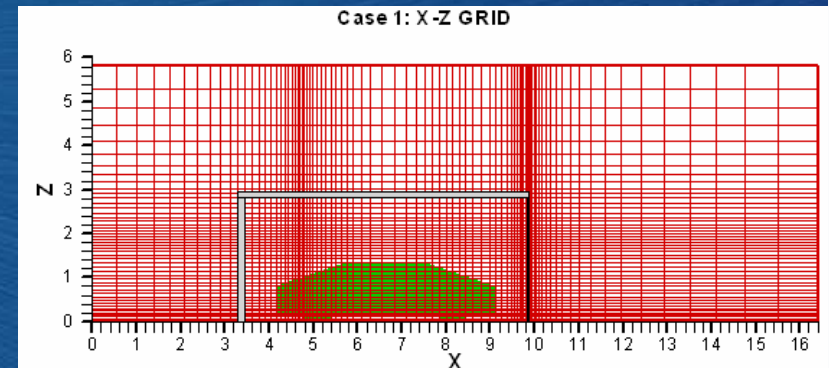


CFD Simulations – Helium release in a private garage (4)

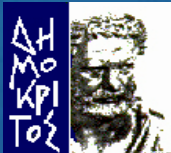
(ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

Computational Grid

- 3-D Cartesian grid
- Grid refinement close to vents, source, walls
- Max. grid expansion ratio: 1.2
- Min. grid expansion ratio: 0.84
- Classification of cells into fully active, inactive and partially active
- DELTA_B Code for geometrical pre-processing



Grid characteristics	Case 1	Case 2	Case 3
Grid dimensions	88×26×48	88×26×50	88×26×44
Number of active cells	101.887	106.218	93.552
Min. and Max. cell size in z-direction (m)	0.04 close to source 0.512 at domain's top	0.038 close to source 0.513 at domain's top	0.065 close to source 0.516 at domain's top
Min. and Max. cell size in x-direction (m)	0.02 close to door 0.92 at domain's end		
Minimum and Maximum cell size in y-direction (m)	0.1 close to source and symmetry plane 0.401 at domain's beginning		

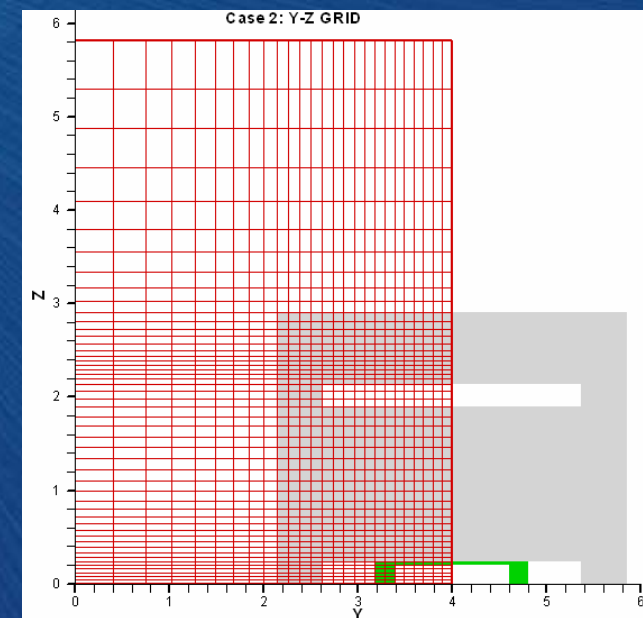
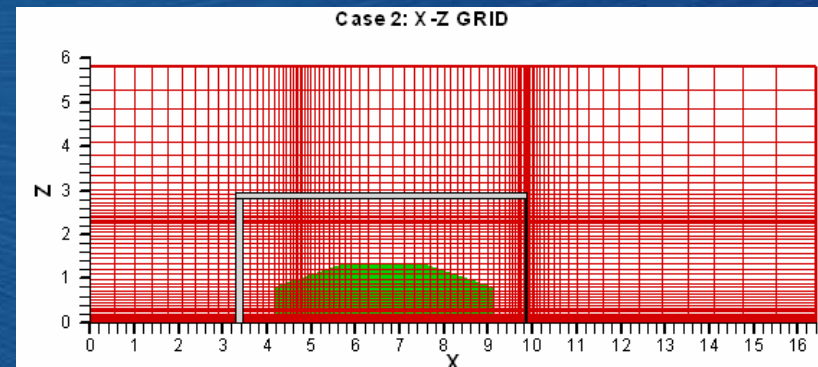


CFD Simulations – Helium release in a private garage (5)

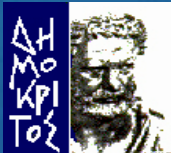
(ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

Computational Grid

- 3-D Cartesian grid
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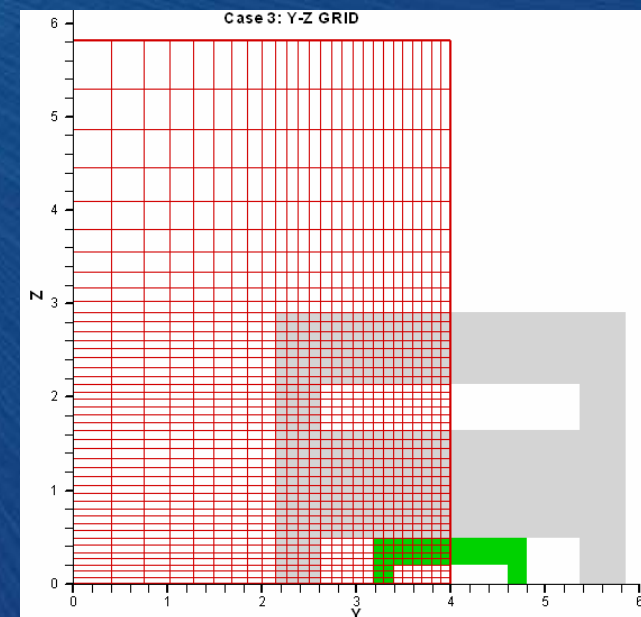
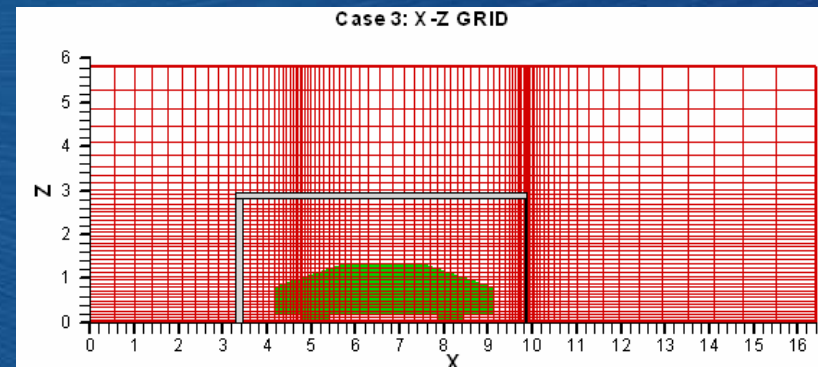


CFD Simulations – Helium release in a private garage (6)

(ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

Computational Grid

- 3-D Cartesian grid
- Grid refinement close to vents, source, walls
- Max. grid expansion ratio: 1.2
- Min. grid expansion ratio: 0.84
- Classification of cells into fully active, inactive and partially active
- DELTA_B Code for geometrical pre-processing



Grid characteristics	Case 1	Case 2	Case 3
Grid dimensions	88×26×48	88×26×50	88×26×44
Number of active cells	101.887	106.218	93.552
Min. and Max. cell size in z-direction (m)	0.04 close to source 0.512 at domain's top	0.038 close to source 0.513 at domain's top	0.065 close to source 0.516 at domain's top
Min. and Max. cell size in x-direction (m)	0.02 close to door 0.92 at domain's end		
Minimum and Maximum cell size in y-direction (m)	0.1 close to source and symmetry plane 0.401 at domain's beginning		



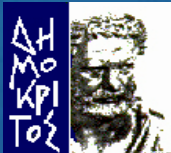
CFD Simulations – Helium release in a private garage (7) (ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

Mathematical Formulation

- 3-D transient, fully compressible conservation equations
 - Mixture mass
 - Mixture momentum
 - Helium mass fraction
 - Mixture density and mass fractions
- Component densities through ideal gas law
- Standard k- ϵ model for turbulence

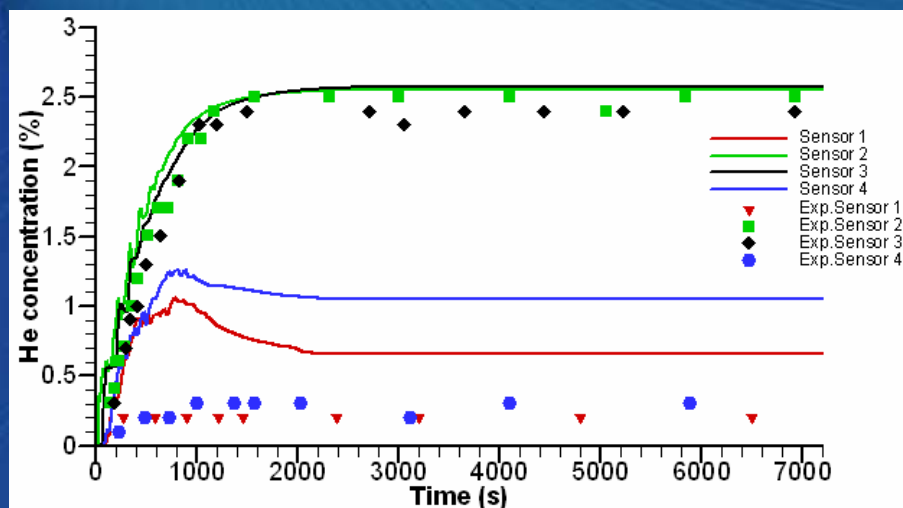
Initial Conditions

- Zero wind velocity with no turbulence
- Temperature of 293.15 K and hydrostatic pressure



CFD Simulations – Helium release in a private garage (8) (ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

Results

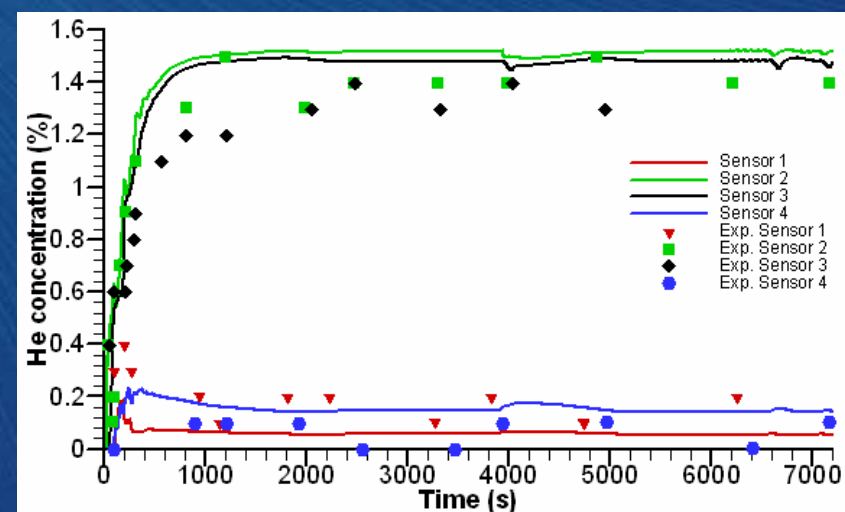


Case 1 (2.5 inches)

- Good agreement for sensors 2 and 3 (upper vent)
- Overestimation for sensors 1 and 4 (lower vent)
- Underestimation of the predicted concentration difference between top and lower sensors

Case 2 (9.5 inches)

- The vent sizes are almost 4 times broader than in Case 1
- The predicted He concentrations are in satisfactory agreement with the experimental data for all sensors



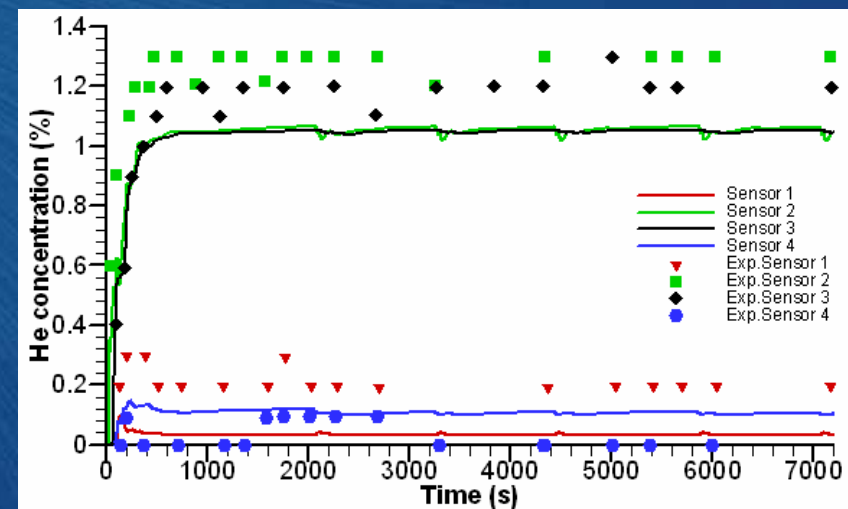


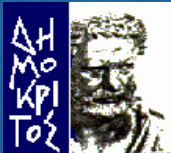
CFD Simulations – Helium release in a private garage (9) (ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

Results

Case 3 (19.5 inches)

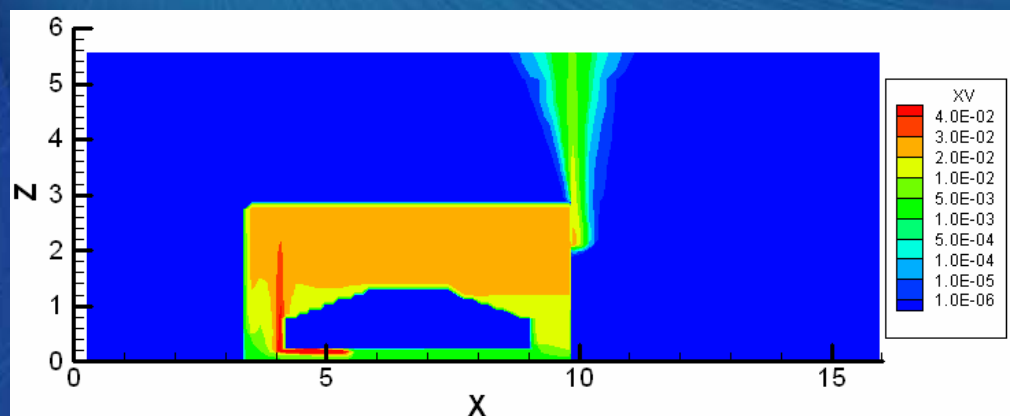
- Underestimation for sensors 1, 2 and 3
- Small over prediction for sensor 4
- The predicted natural ventilation rate is overestimated



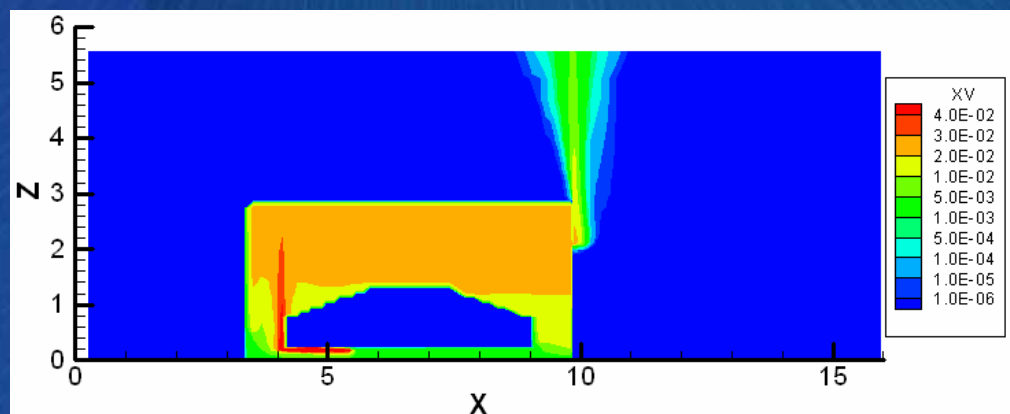


CFD Simulations – Helium release in a private garage (10) (ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

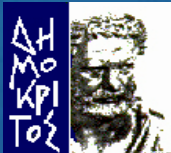
Results



**He vol. concentration contours
(XV) in x-z symmetry plane at
t = 3.600 sec**

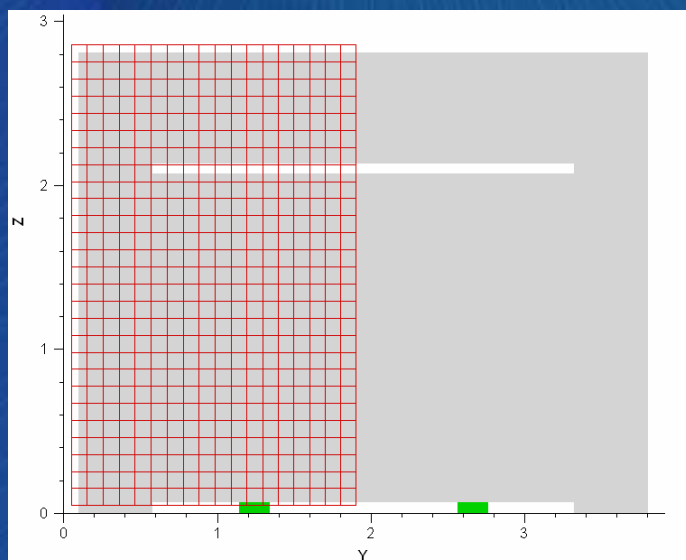
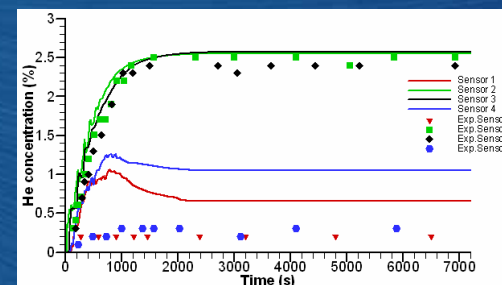
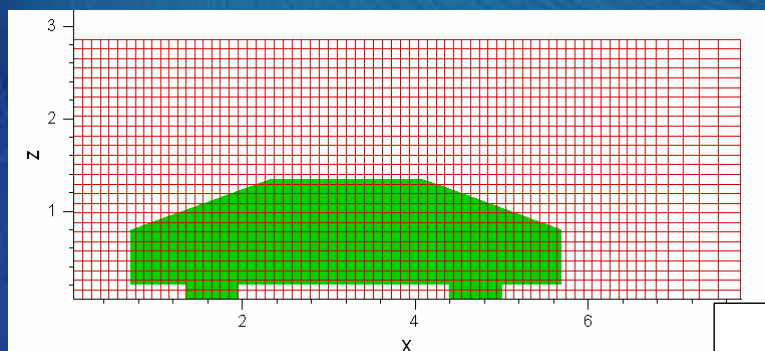


**He vol. concentration contours
(XV) in x-z symmetry plane at
t = 7.200 sec**

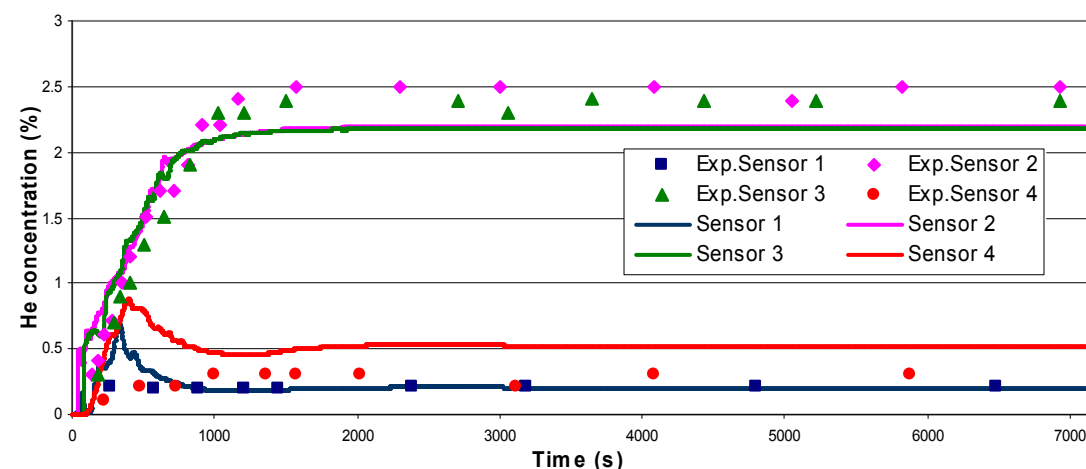


CFD Simulations – Helium release in a private garage (11) (ICHS, Pisa, Sept 2005 and 2nd ELETY, Thessaloniki, Oct 2005)

New Simulations (change of grid)



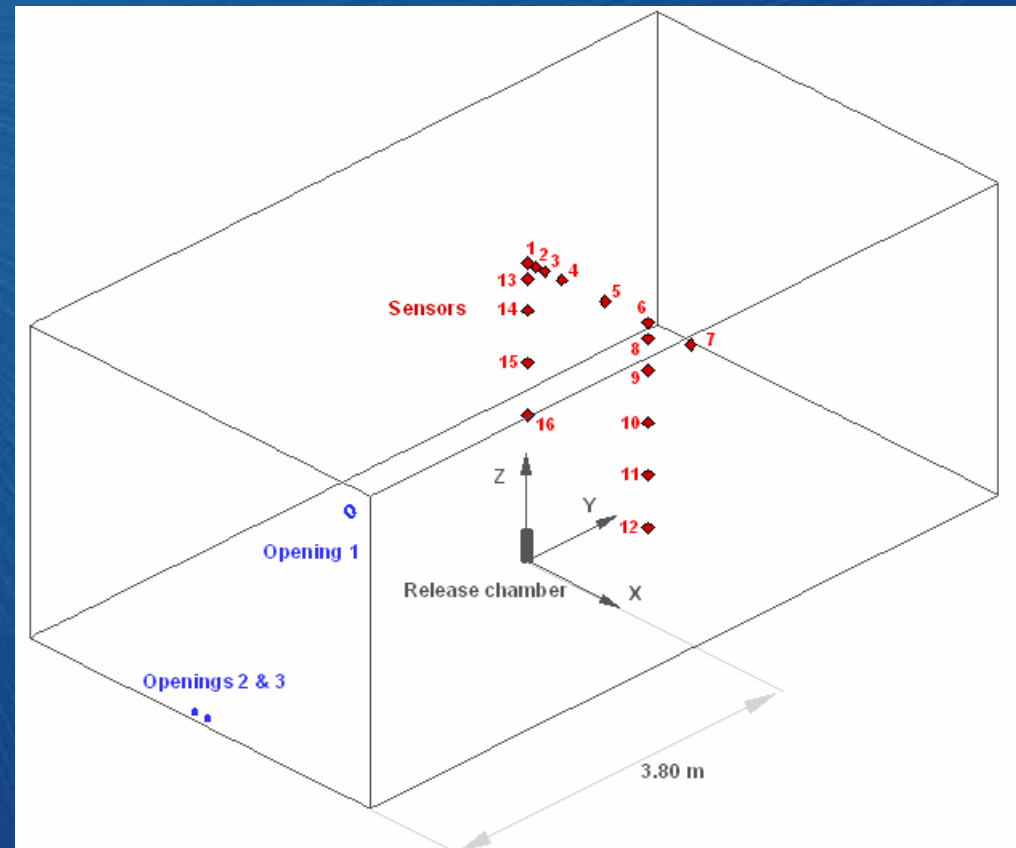
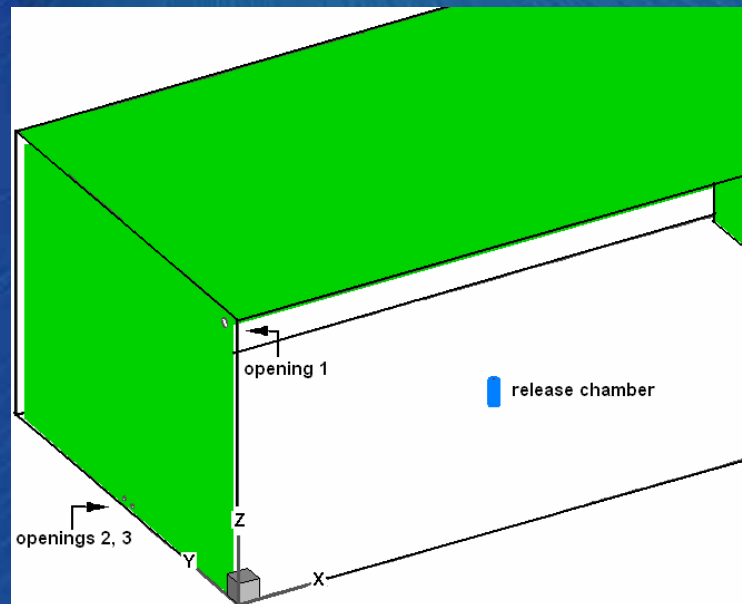
Case 1: 2.5 inches top and bottom vents



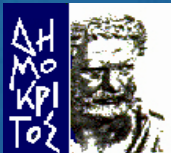


CFD Simulations – InsHyde Project (1)

H₂ release from bottom of chamber directed upwards



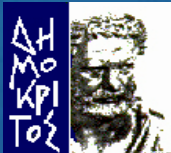
Experimental facility with sensor locations



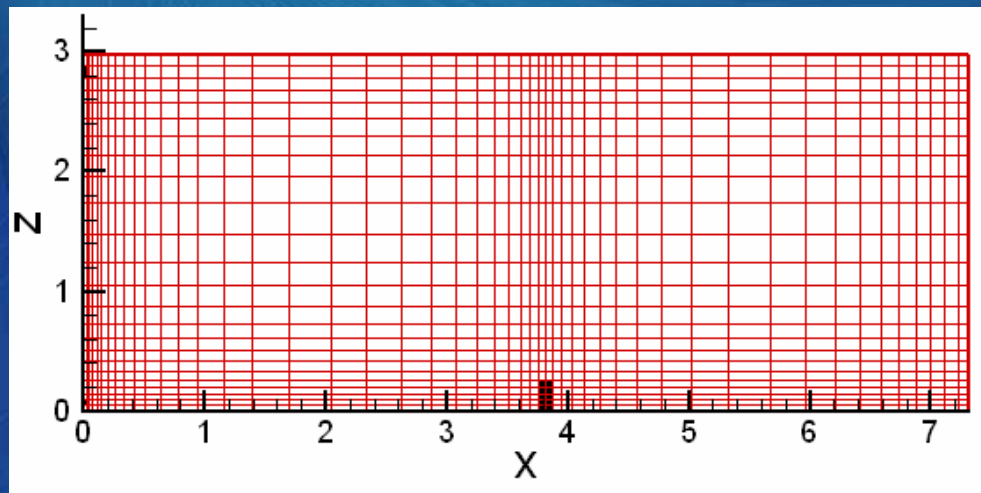
CFD Simulations – InsHyde Project (2)

Pre-tests calculations

Case 1	Simulation duration: 600 s	Release flow rate: 5 mg/s, Release duration: 600 s, Orifice diameter: 10 mm Natural ventilation
Case 2	Simulation duration: 600 s	Release flow rate: 5 mg/s, Release duration: 600 s, Orifice diameter: 20 mm Natural ventilation
Case 3	Simulation duration: 600 s	Release flow rate: 100 mg/s, Release duration: 600 s, Orifice diameter: 20 mm Natural ventilation
Case 4	Simulation duration: 600 s	Release flow rate: 100 mg/s, Release duration: 600 s, Orifice diameter: 20 mm Forced ventilation: 240 m ³ /h, Simultaneous forced ventilation and release
Case 5	Simulation duration: 240 s	Release flow rate: 1.000 mg/s, Release duration: 240 s, Orifice diameter: 4 mm Natural ventilation
Case 6	Simulation duration: 240 s	Release flow rate: 1.000 mg/s, Release duration: 240 s, Orifice diameter: 20 mm, Natural ventilation
Case 6_b	Simulation duration: 3.000 s	Release flow rate: 1.000 mg/s, Release duration: 240 s, Orifice diameter: 20 mm Natural ventilation
Case 7	Simulation duration: 240 s	Release flow rate: 100 mg/s, Release duration: 240 s, Orifice diameter: 20 mm Forced ventilation: 240 m ³ /h, Pre-existing forced ventilation for 200 s



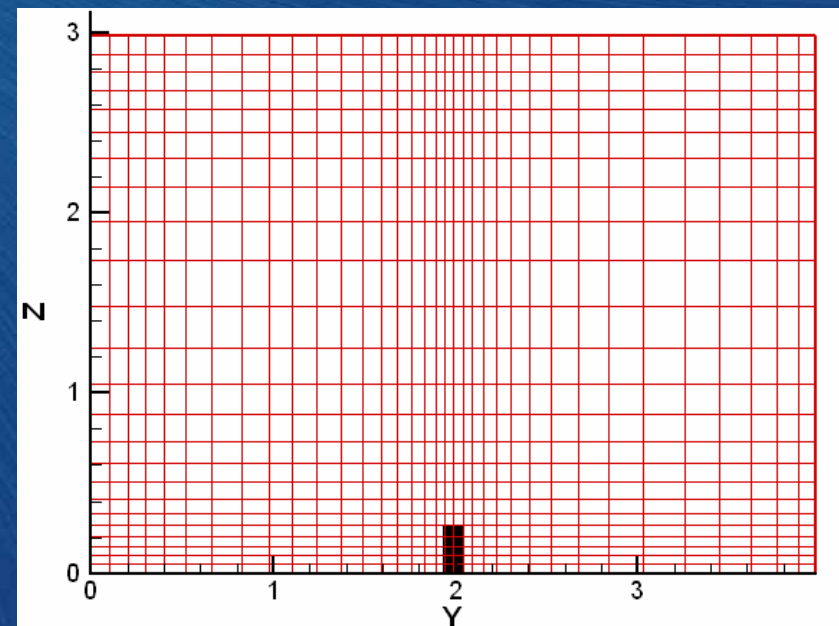
CFD Simulations – InsHyde Project (3)



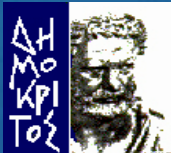
x-z computational grid

Turbulence modeled with
k- ϵ model

Computational cells 36.000

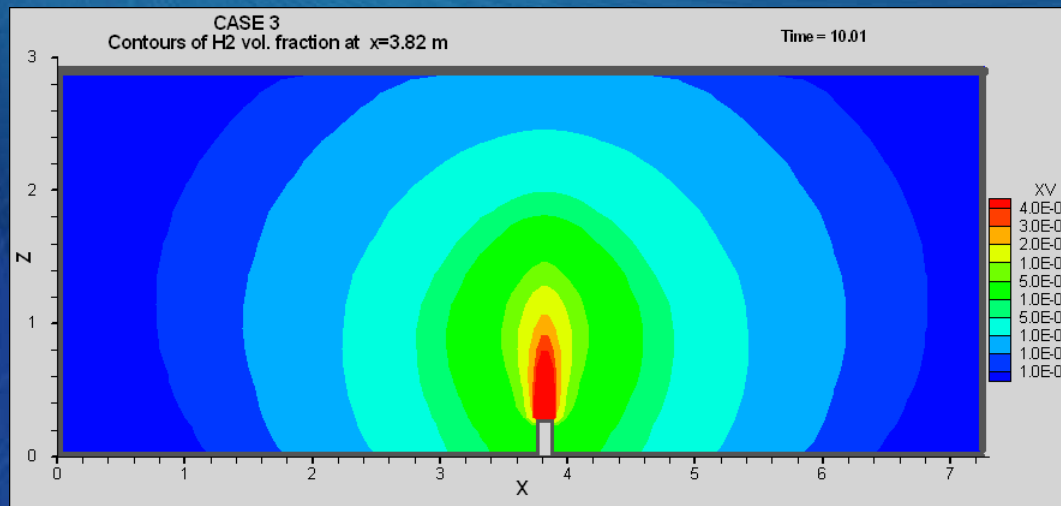


y-z computational grid

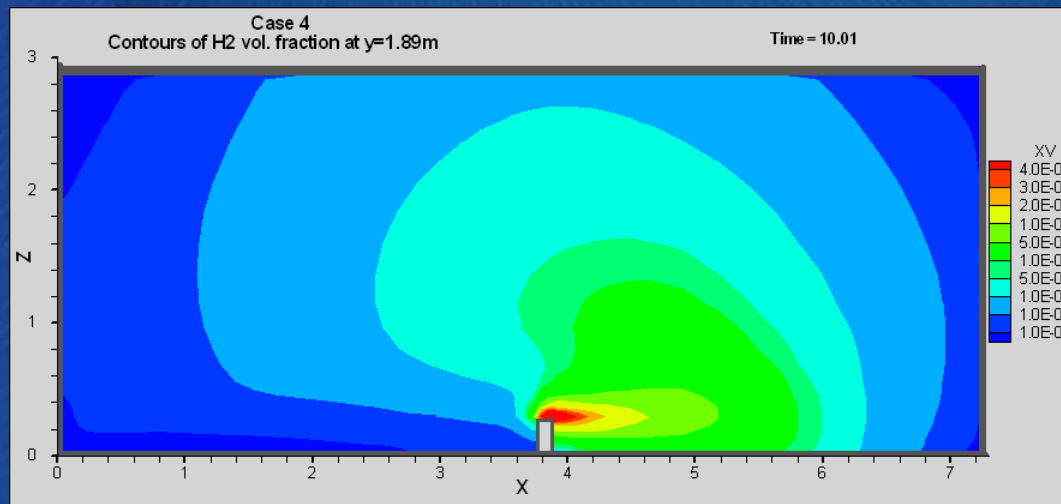


CFD Simulations – InsHyde Project (4)

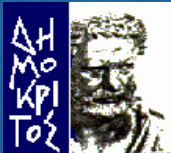
Adrea-HF predictions



Case 3
(0.1 kg/s for 600 seconds,
natural ventilation)

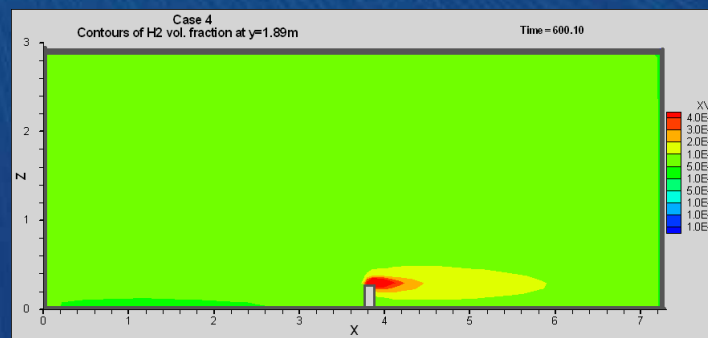
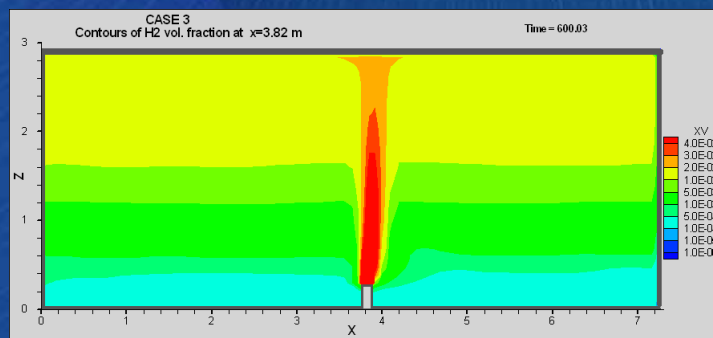
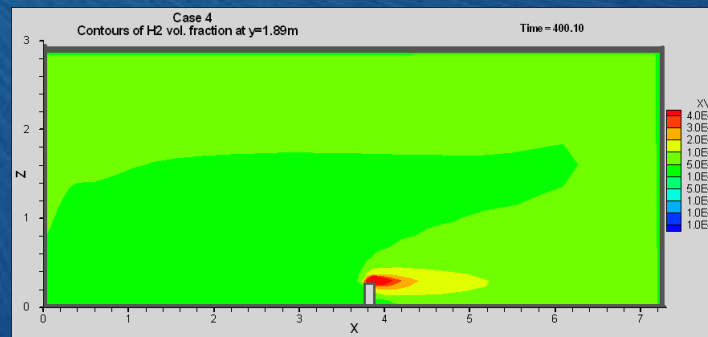
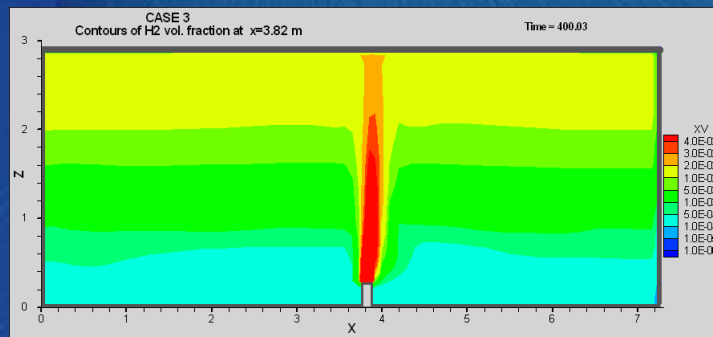
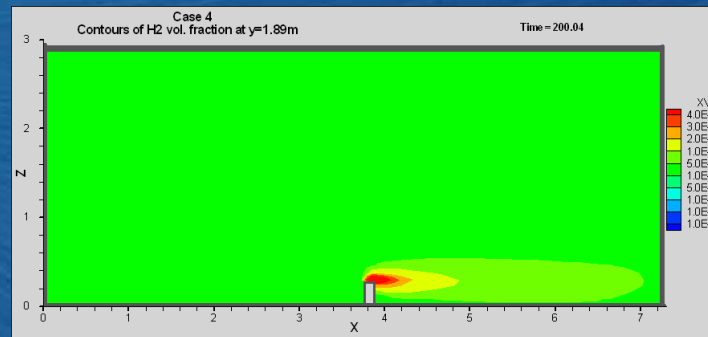
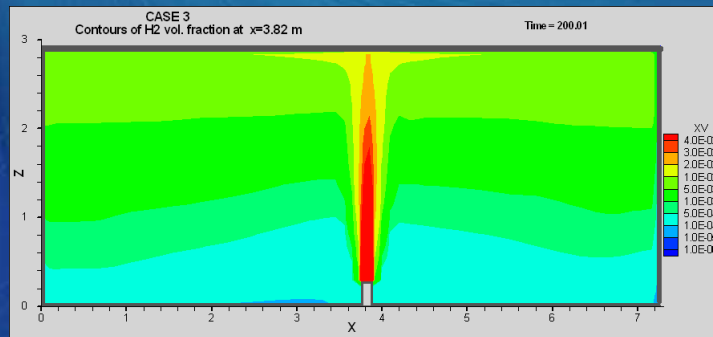


Case 4
(0.1 kg/s for 600 seconds,
forced ventilation-240 m³/h)



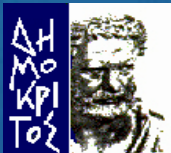
ΗΜΕΡΙΔΑ ΥΠΟΤΡΟΦΩΝ ΙΠΤΑ
ΔΗΜΟΚΡΙΤΟΣ
28/03/07

CFD Simulations – InsHyde Project (5)



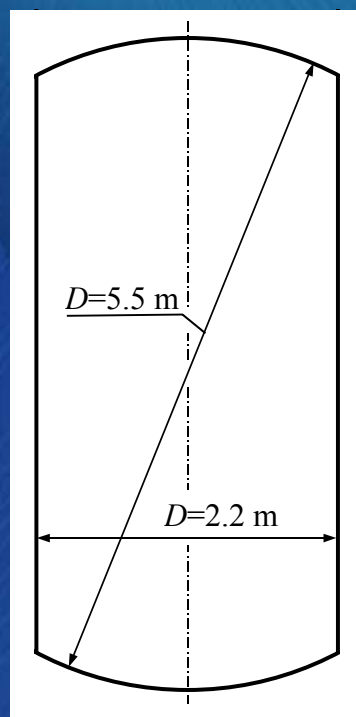
Adrea-HF predictions

Case 3 and Case 4 are completely different. The ventilation flow rate of 3 ACH of Case 4 creates strong recirculation which in turn causes a very rapid mixing inside the chamber. It can be observed clearly from the movies that even at about 80 seconds the chamber contains a homogenous air/H₂ mixture i.e. no stratification is present.



CFD Simulations – HySafe Project (1)

Subsonic release of hydrogen into 20 m³ closed vessel within 60 seconds with consequent mixing and distribution during time up to 250 minutes



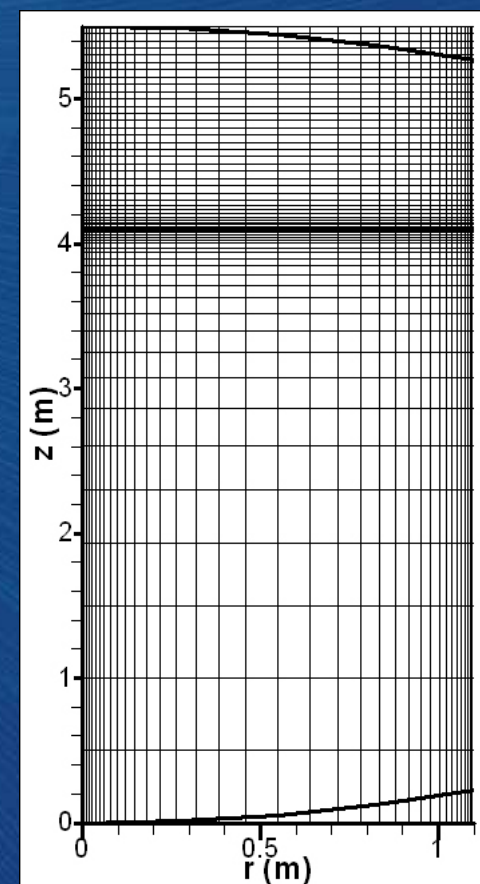
Vessel
geometry for
simulations

Experimental Description

Hydrogen is released 1.4 m below the top of the vessel vertically upward, 4.5 litres per second during 60 seconds (0.27 m³ totally). Taking into account that in experiment the tube diameter was 10 mm, it corresponds to the hydrogen release velocity 57.3 m/s.

Computational domain and grid

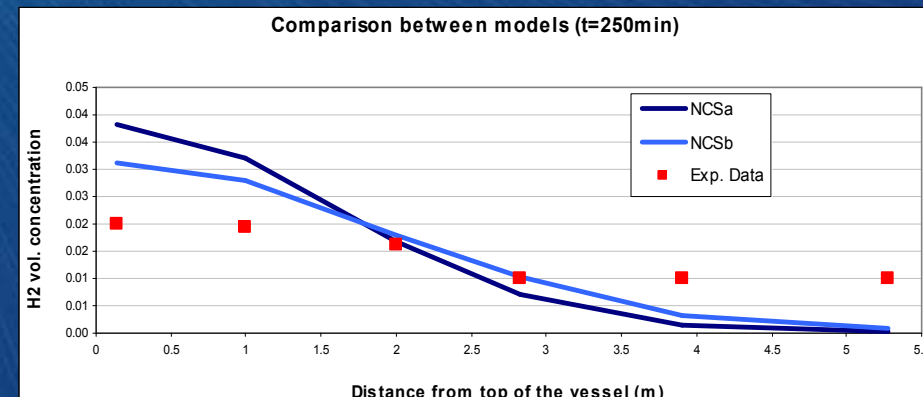
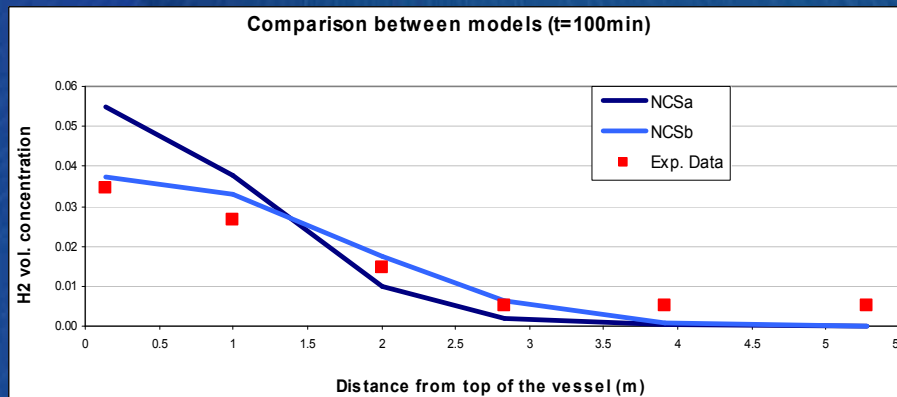
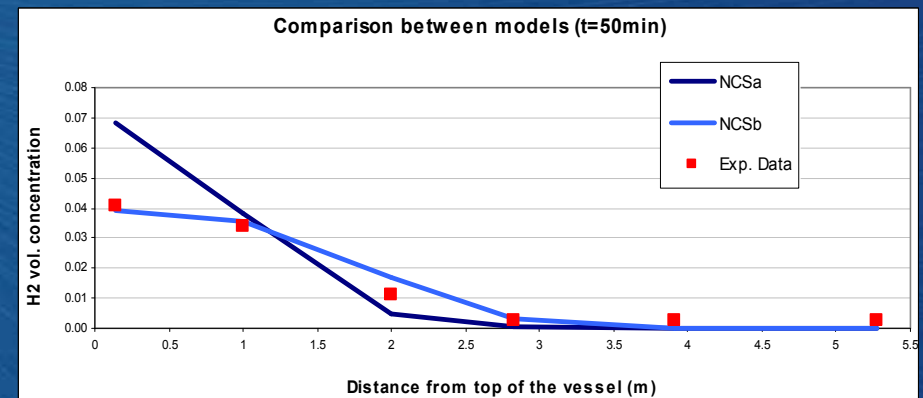
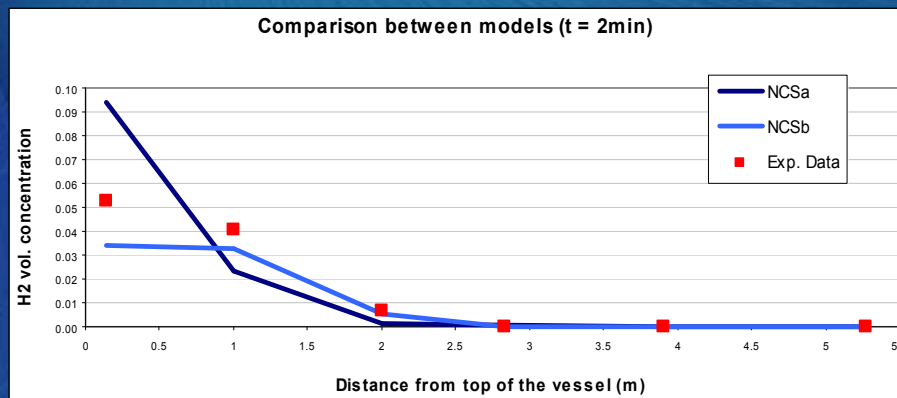
Cylindrical symmetry
assumption
Non-equidistant grid
with 36x61 cells
2.071 total number of
cells

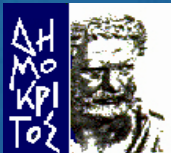




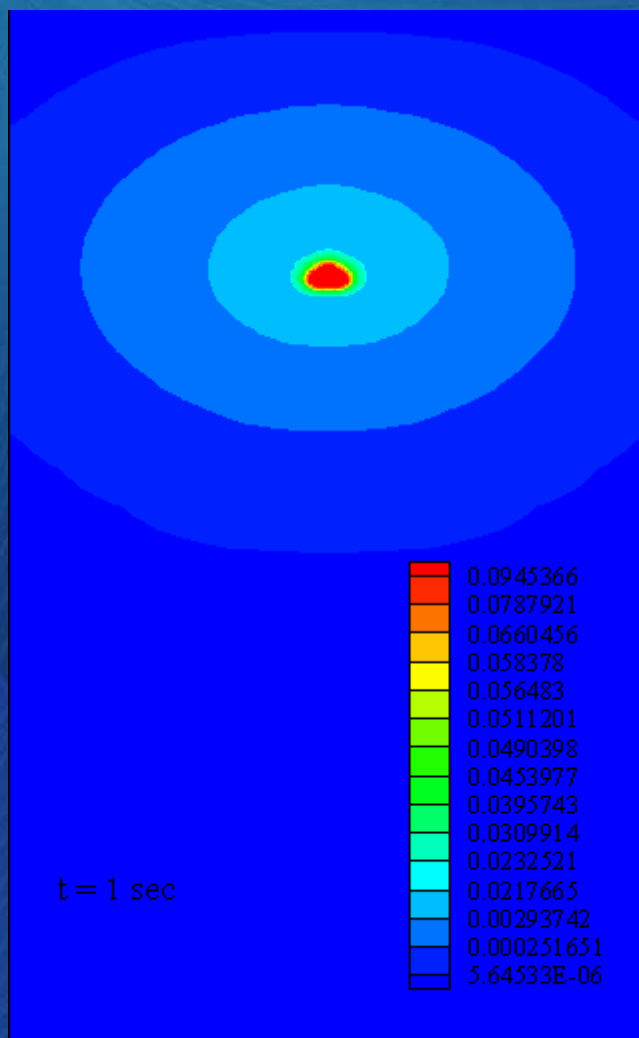
CFD Simulations – HySafe Project (2)

Adrea-HF predictions Models used: Standard k-epsilon (NCSa) and LVEL model (NCSb)

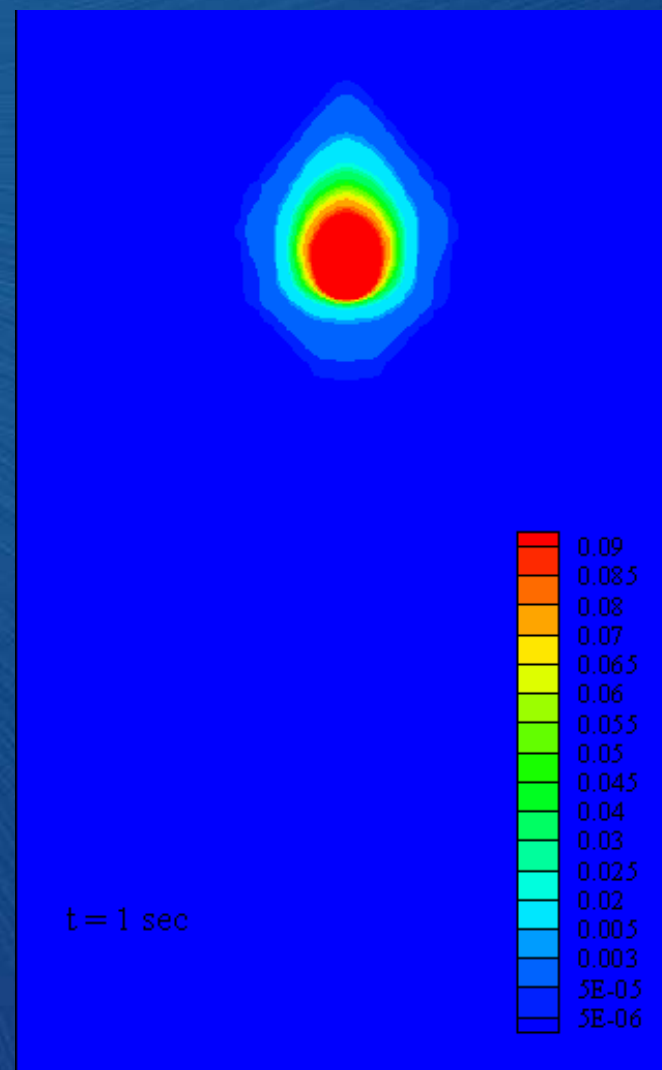




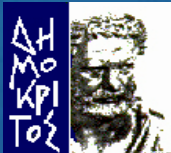
CFD Simulations – HySafe Project (3)



Standard k-epsilon



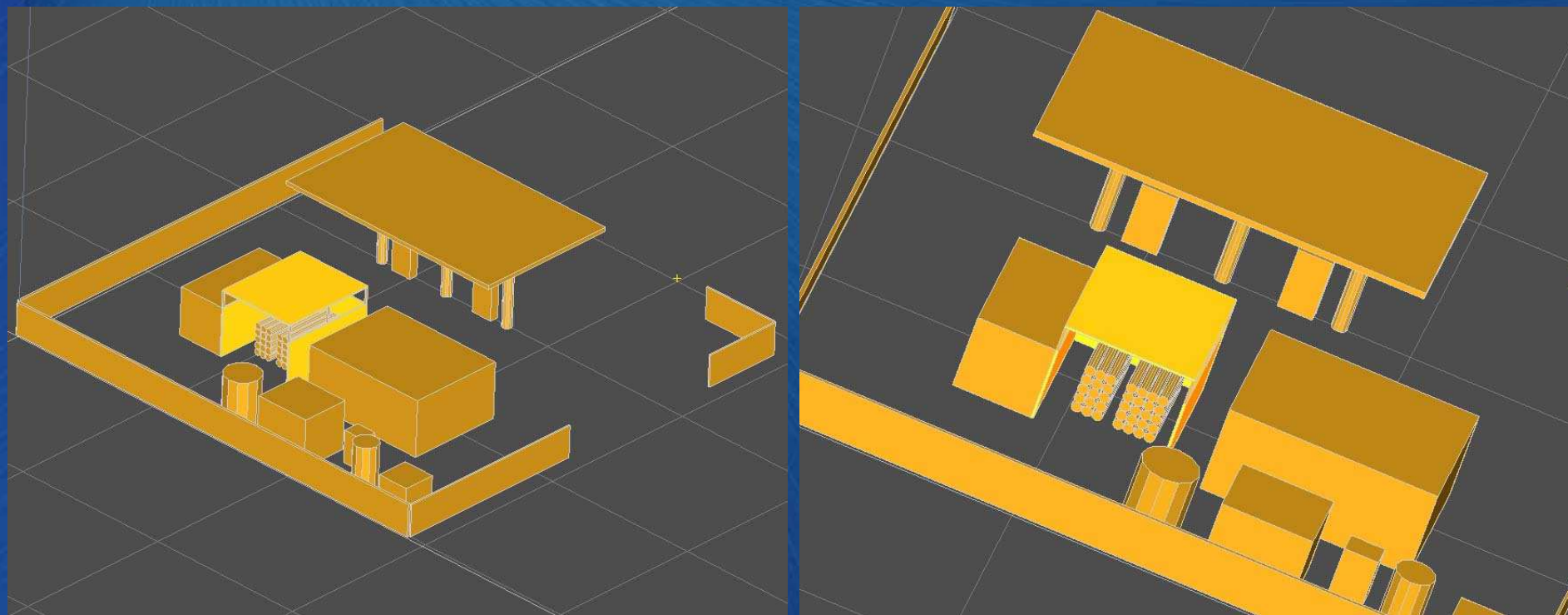
LVEL model



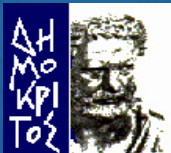
CFD Simulations in progress

Experimental description (Tanaka et. al. 2005)

Full-Scale Hydrogen Filling Station dispersion and explosion experiments
Release of Hydrogen at high pressure (10 MPa) using small nozzle sizes (0.8-1.6 mm)



Aspects of the site geometry to be simulated



• Publications and Presentations

■ Publication to an international scientific journal

Gallego, E., Migoya, E., Martin-Valdepenas, J.M., Crespo, A., Garcia, J., Venetsanos, A., Papanikolaou, E., Kumar, S., Studer, E., Hansen, O.R., Dagba, Y., Jordan, T., Jahn, W., Hoiset, S., Makarov, D. and Piechna, J.
“An Intercomparison Exercise on the Capabilities of CFD Models to Predict Distribution and Mixing of H₂ in a Closed Vessel”, submitted for publication to the International Journal of Hydrogen Energy

■ Presentation at the *International Conference on Hydrogen Safety (ICHS)*, September 8-10, 2005, Pisa, Italy

Papanikolaou, E.A. and Venetsanos, A.G., “CFD Modelling for Helium Releases in a Private Garage without Forced Ventilation”

■ Presentation at the *2nd National Conference for Hydrogen Technologies*, 20-21 October, 2005, Thermi, Thessaloniki, Greece

Papanikolaou, E.A. and Venetsanos, A.G., “CFD Modelling for Hydrogen Releases in a Private Garage without Forced Ventilation”

• Current Research Projects

■ HYSAFE Network of Excellence (Funded under EC): “Safety of Hydrogen as an Energy Carrier”

- INSHYDE: “internal project - release in (partially) confined areas”
- HyTunnel

■ HyApproval: “Handbook for Approval of Hydrogen Refueling Stations (under EC)”

■ Hyper (Co-funded under EC): “Installation Permitting Guidance for Hydrogen and Fuel Cells Stationary Applications”