The ADREA-HF CFD code
An overview

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Computational Fluid Dynamics (CFD)

- It is well known that CFD is increasingly applied for consequence assessment studies and Regulation Codes and Standards (RCS) support
- Main reasons:
  - CFD has the ability to treat complex scenarios, which simpler integral tools cannot handle
  - CFD cost is relatively lower than experiments
  - CFD tools present generally realistic simulation times
  - CFD tools/models are increasingly validated against relevant release, dispersion and combustion phenomena

ADREA-HF code Scope

- CFD prediction of flow and dispersion of pollutants in complex geometry at local scale for consequence assessment of accidental releases under realistic conditions
- With applications in
  - Chemical industry
  - Petrochemical industry
  - Automotive industry
  - Hydrogen technologies
  - RCS support
  - CO_2 technologies …

ADREA-HF code Physics-1

- The fluid
  - Ideal multi-component mixtures
  - Thermodynamic equilibrium (HEM)
  - Each specie can be in vapor or non-vapor phase (water or solid)
  - Solidification modelling following Witlox et al., JLP, 2009
  - Raoult's law to obtain non-vapor fractions
  - User specified physical properties (non-ideal gas physical properties from tables)
- The mean flow
  - Solves the 3d, time dependent fully compressible conservation equations for mixture mass, momentum, enthalpy and total component mass (one for each component)
  - Hydrodynamic non-equilibrium (slip velocity between phases)
- Turbulence
  - RANS turbulence modelling. Series of turbulence models.
  - Pollutant concentration fluctuations modeled
  - LES modelling (Smagorinski, RNG)
  - Various turbulent Prandtl number models

ADREA-HF code Physics-2

- Boundary conditions
  - Solid air thermal interaction by solving the 1d temperature equation inside the ground
  - Various wall function capabilities (account of stability)
- Pollutant Sources
  - Handles dense, neutral and buoyant releases.
  - Instantaneous and time-varying (continuous) releases.
  - Subsonic and sonic jets.
  - Single and two-phase releases
  - Pool formation and spreading modelled
- Combustion
  - Eddy dissipation model (currently under validation for CH_4 and H_2 combustion)

ADREA-HF code — Numerics

- Discretization
  - Control volume approach in Cartesian grids
  - Solids/obstacles treated with porosity formulation
- Accuracy
  - Up 3^{rd} order for convective terms (high order schemes with limiters)
  - Up to 2^{nd} order in time (Crank Nickolson or backwards Euler)
- Solution techniques
  - Bi-CGStab and GMRES solvers
  - various types of pre-conditioners giving computing time nearly O(N)
  - Parallel calculations with OpenMP for shared memory machines
  - Parellel calculations with MPICH for clusters and/or shared memory machines
  - Automatic time step increase/decrease procedures

ADREA-HF code — Numerics

- User specific
  - No memory restrictions. Full dynamic memory allocations.
  - Run can be stopped and restarted from where it stopped
  - Run can read and interpolate results from previous ADREA-HF run on different grid
  - User can write his own FORTRAN code and have access to the ADREA-HF internal code variables. User routines are called at the beginning of run and at end of each time step

ADREA-HF code GUI

- Environment
  - GUI in Windows (OpenCascade based)
  - Main code (VC++ and F90) in Windows and Linux
- Pre-processing
  - Fast geometry introduction (primitive shapes, complex shapes, boolean operations between solids)
  - Import of geometry from (IGES, STEP, BREP, CSFDB)
  - Export of geometry to (IGES, BREP, STL, VRML, TECPLOT)
- Post-processing
  - Contours, vectors, iso-surfaces
  - Export to TECPLOT

ADREA-HF code Validation

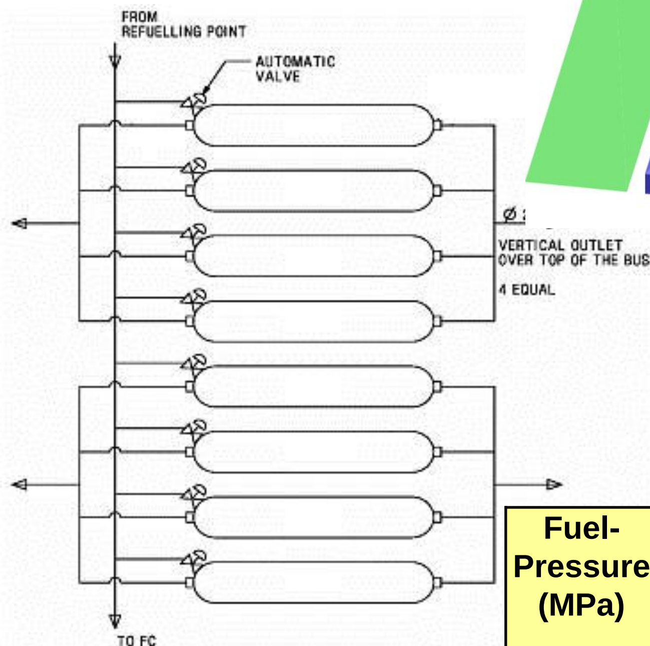
- Dense gas
  - Thorney island 8 and 21. Instantaneous releases of Fr/N2 mixture without and with circular fence
  - EMU-C1 continuous Cl release in a chemical plant
- Passive
  - EMU-A1 continuous release from the door of L-shape building
- Subsonic buoyant jets
  - Russian-2 H2 jet in $20m^3$ hermetically sealed cylinder
  - INERIS-6C H2 jet in $78m^3$ garage like gallery
  - Swain garage. He jet in $67m^3$ private parking with vehicle
  - GEXCON-D27 H2 jet in $0.2m^3$ compartmented enclosure
- Sonic buoyant jets
  - FZK tests. H2 jets at 100 and 160bar
  - HSL-7. H2 jet at 100bar
  - Osaka HRS. H2 jets at 400bar in the storage room of the Osaka H2 refuelling station
- Two-phase jets
  - EEC-55. C3H8 release on flat ground with and without fence
  - Burro 9 LNG release on water
  - Falcon-1 LNG release in complex geometry
  - Desert Tortoise 1. NH3 release on flat ground
  - BAM-5. LH2 release within buildings
  - NASA-6. LH2 release on flat ground with circular fence

ADREA-HF code — Projects

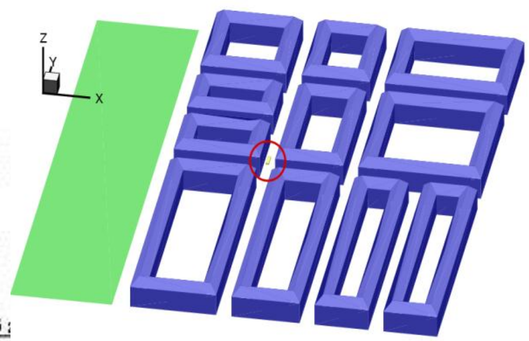
- EIHP project (FP5)
  - H_2 releases from private cars in tunnel
- EIHP2 project (FP5)
  - H_2 releases from H_2 bus in city and tunnel environments. Comparison to NG releases from NG bus
- Hong Kong project (Private Contract)
  - H_2 releases from H_2 bus in Hong Kong
- HYSAFE project (FP6, NoE)
  - H_2 releases validation
- HYAPPROVAL project (FP6, STREP)
  - H_2 releases from hydrogen refuelling stations
- HYPER project (FP6, STREP)
  - H_2 releases from fuel cells in confined ventilated spaces
- CO2PipeHaz project (FP7, Collaborative)
  - CO_2 Physical properties (MTMML)
  - CFD pre-calculations and validation (EREL)

EIHP2 project: CGH2 bus in a city

Release of 40 kg H2 (168 kg CH4) through 4 outlet vents at the top of the bus (Stockholm accident site)

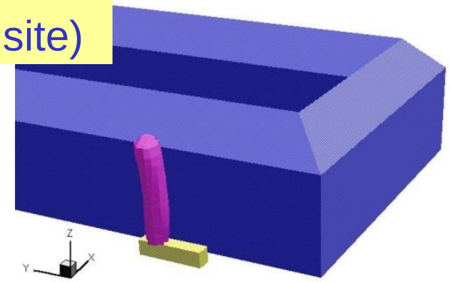


Bus storage system

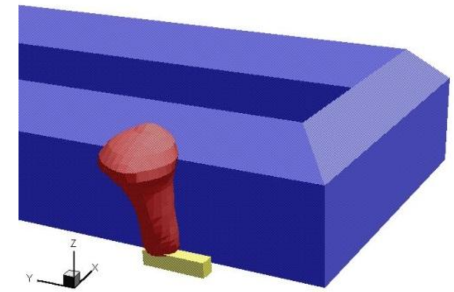


Urban site (Stockholm) showing assumed bus location

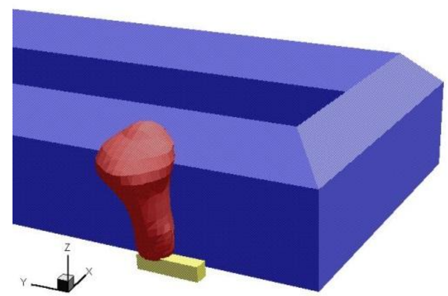
LFL clouds



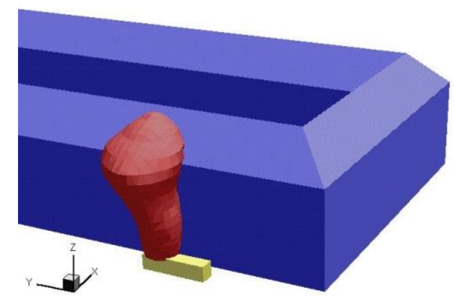
CH4, 20MPa, 7.9s



H2, 20MPa, 10.9s, 12.1 kg



H2, 35MPa, 7.7s, 14.7 kg



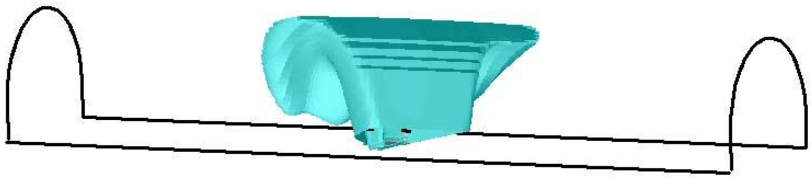
H2, 70MPa, 5.2s, 18.5 kg

Fuel-Pressure (MPa)	Energy (MJ)	Fireball		Overpressure		
		Average diameter at 2.0m above ground (m)	Maximum diameter at any height above ground (m)	Distance to 2kPa overpressure (m)	Distance to 21kPa overpressure (m)	Distance to 35kPa overpressure (m)
H2-20	1460	12.7 [a]	18.8	75	7	3
H2-35	1760	10.5 [a]	15	91	8	3
H2-70	2220	16.0 [a]	21.5	100	9	5
CH4-20	754	11.0 [a]	15	65	L	L

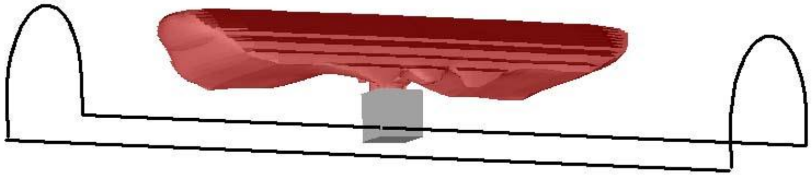
Taken from Venetsanos et al. (2007) J. Loss Prevention in the Process Industry, 21

EIHP2 project: CGH2 bus in tunnel

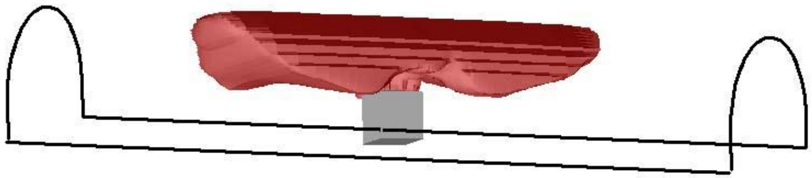
LFL clouds



CH4, 20MPa, 40s, 1756m³, 110kg

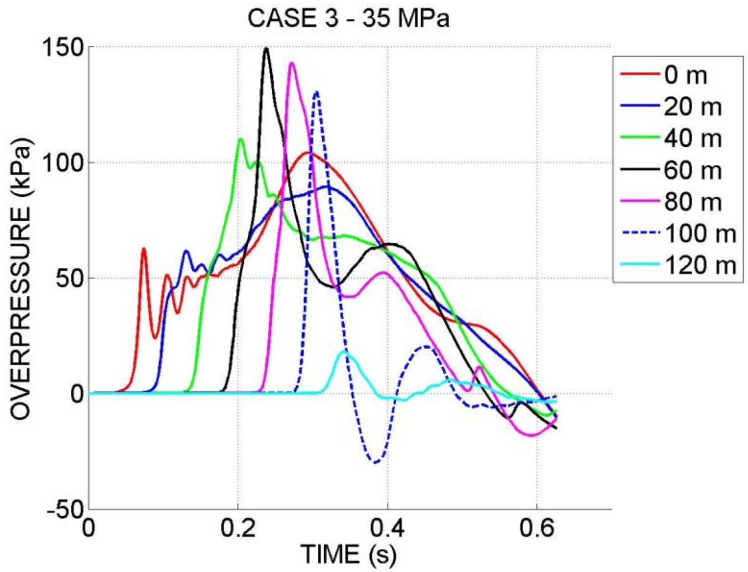


H2, 20MPa, 40s, 2358m³, 32.4kg



H2, 35MPa, 30s, 2180m³, 32.5kg

Release of 40 kg H2 (168 kg CH4) through 4 outlet vents at the top of the bus



FUEL	PRESSURE (MPa)	ENERGY (MJ)	FIREBALL Length Along The Tunnel (m)	OVERPRESSURE Peak Overpressure (kPa)
H2	20	3890	220[a]	42.5
	35	3900	285[a]	150
NG	20	5380	198	45

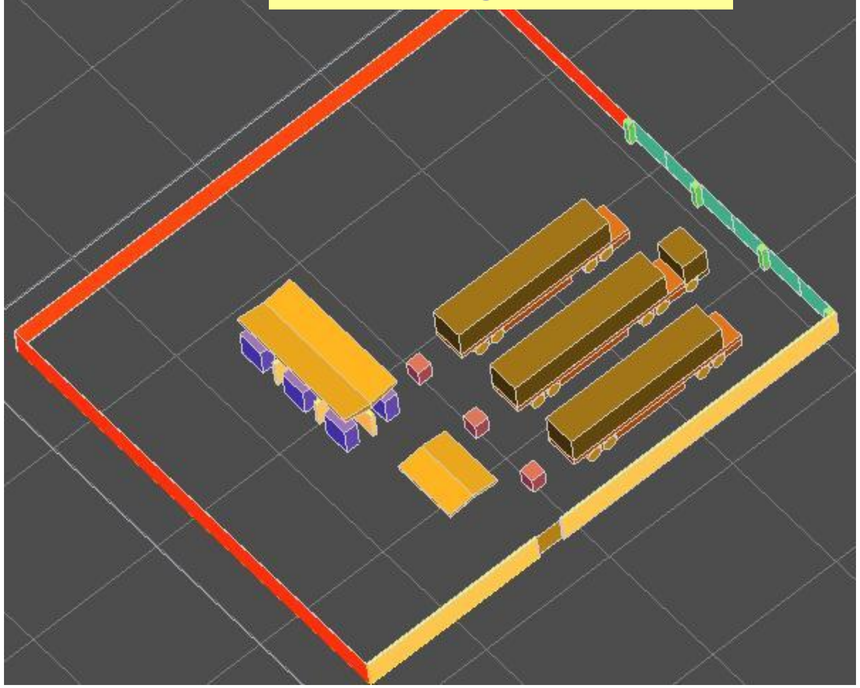
Taken from Venetsanos et al. (2007) J. Loss Prevention in the Process Industry, 21

HyApproval project: Examined scenarios

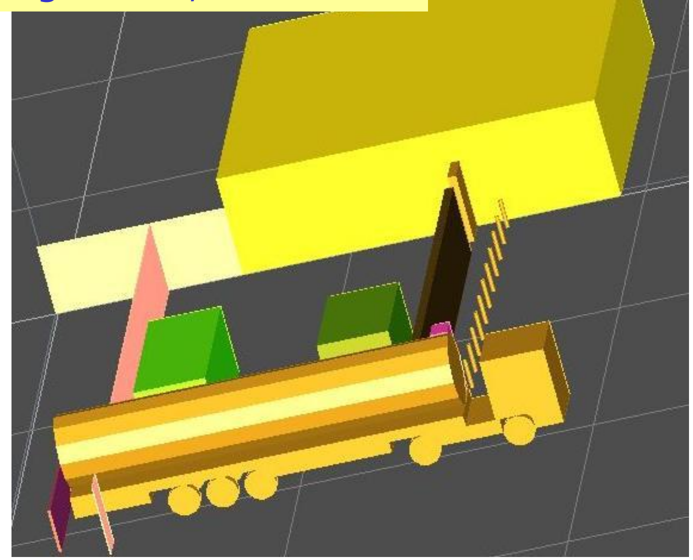
- Dispenser: rupture of dispensing line (CGH2 35 and 70 MPa, LH2)
- Trailer: Hose disconnection during discharge (CGH2 20 MPa, LH2)

Shell-HSL experimental site (2006)

Luxemburg CGH2 site



Washington DC, LH2 site



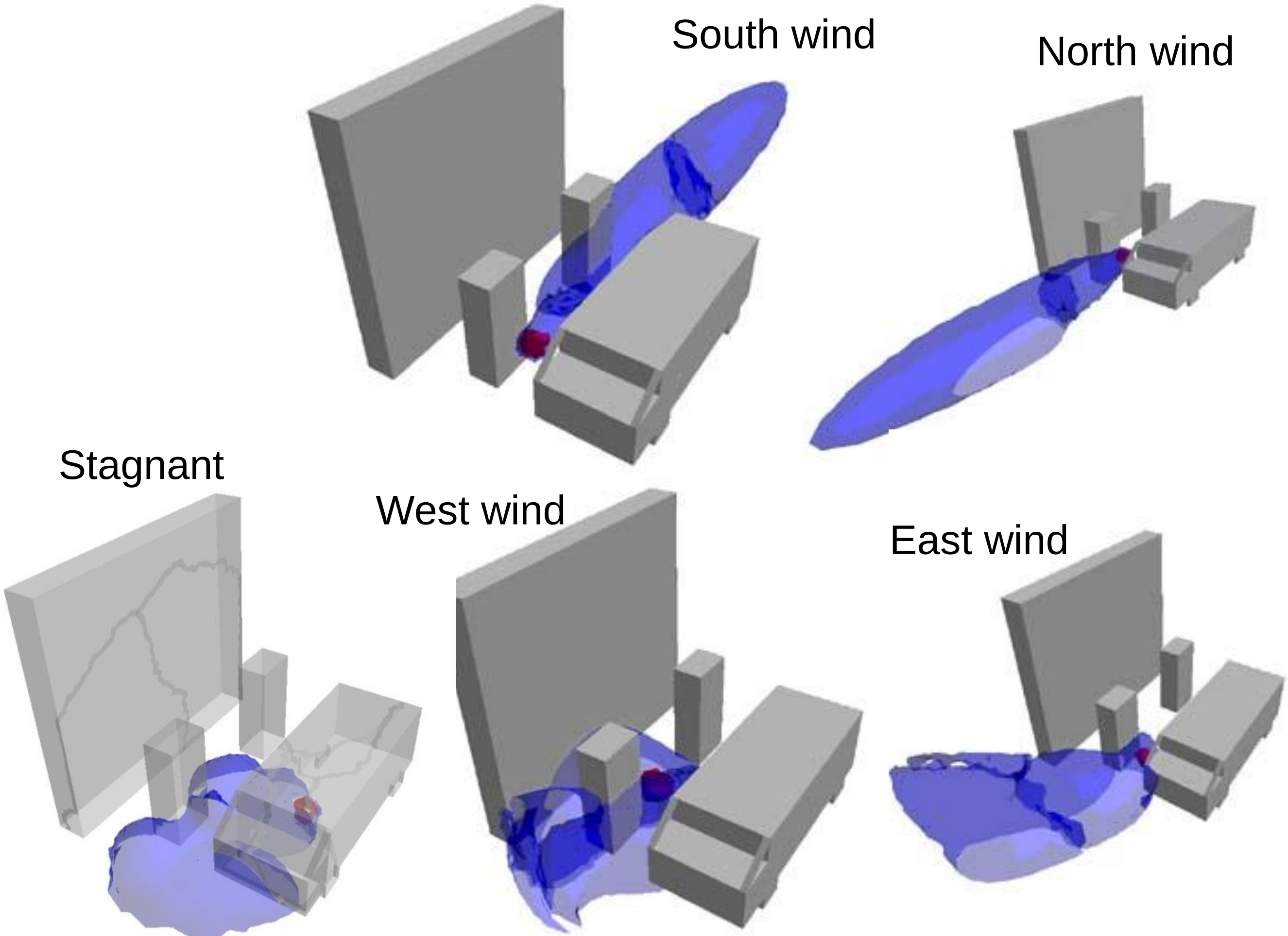
Taken from HyApproval Deliverable 4.6, 2007

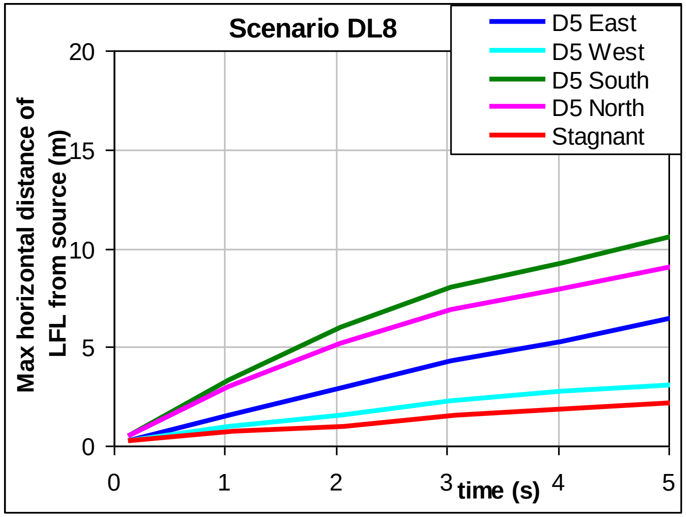
HyApproval project: LH2 dispenser leak

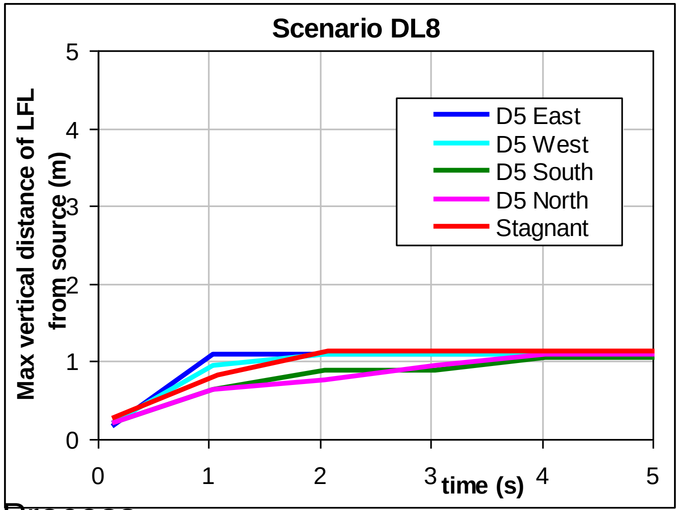
267g LH2 released in 5 seconds (hose id = 8mm)

5 m/s wind at 10m height

Predicted LFL clouds at 5 sec





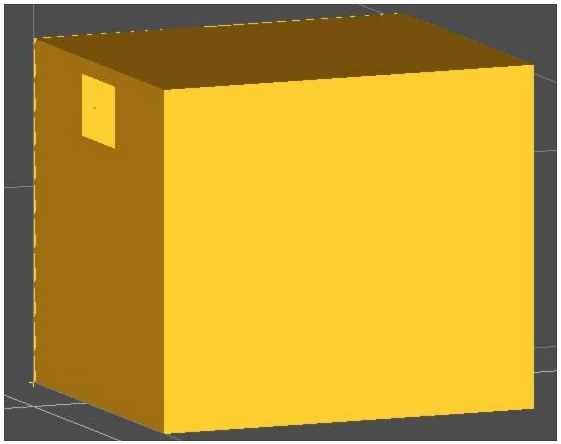


See in Baraldi et al. (2009), Journal of Loss Prevention in the Process Industries (22) 303–315

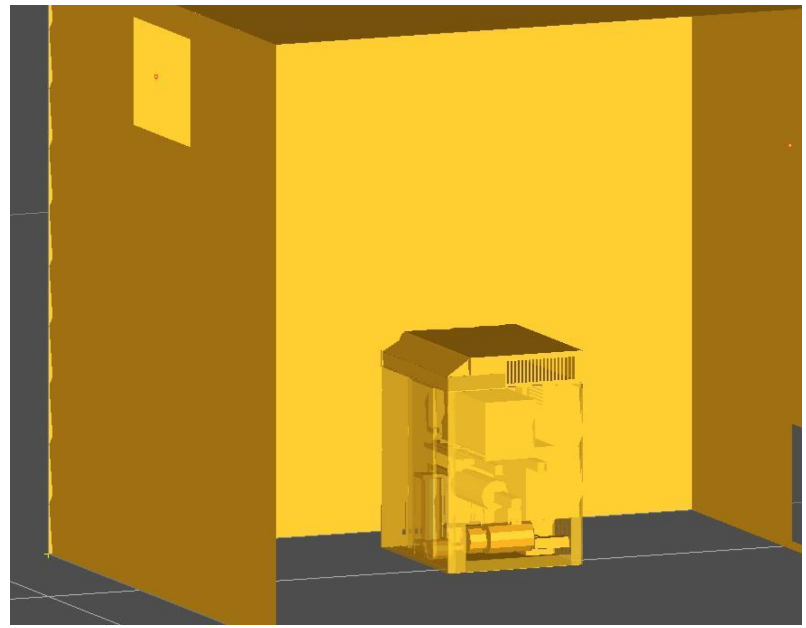
Hyper project: Fuel Cell Leak

Fuel cell located inside naturally ventilated test facility

14.8g H2 released in 60 seconds



Naturally Ventilated Test Facility (CVE)



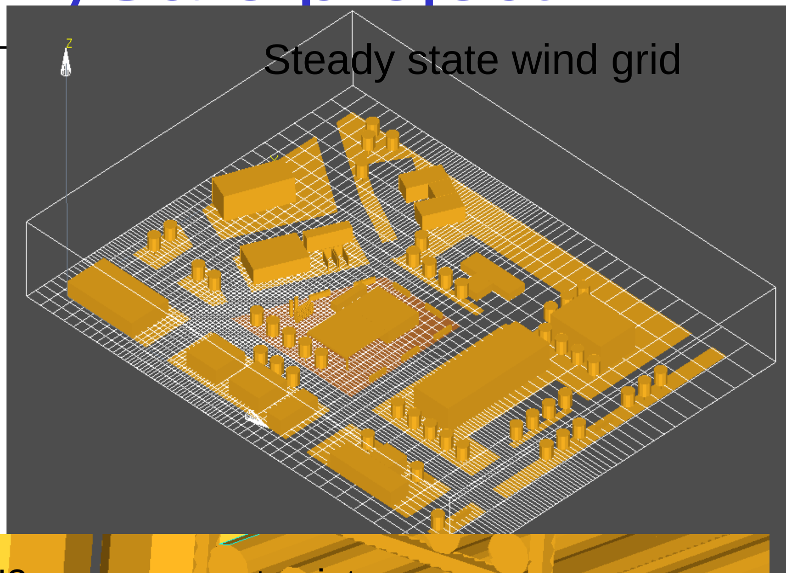
Location and Interior of Fuel Cell

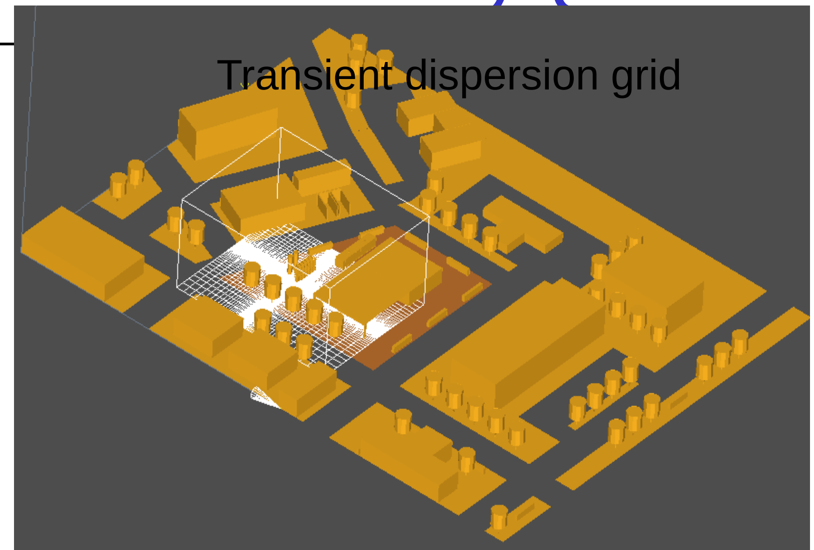
See in Papanikolaou et al. (2011), Int. J. Hydrogen Energy, 36 (2011), pp. 2597-2605.

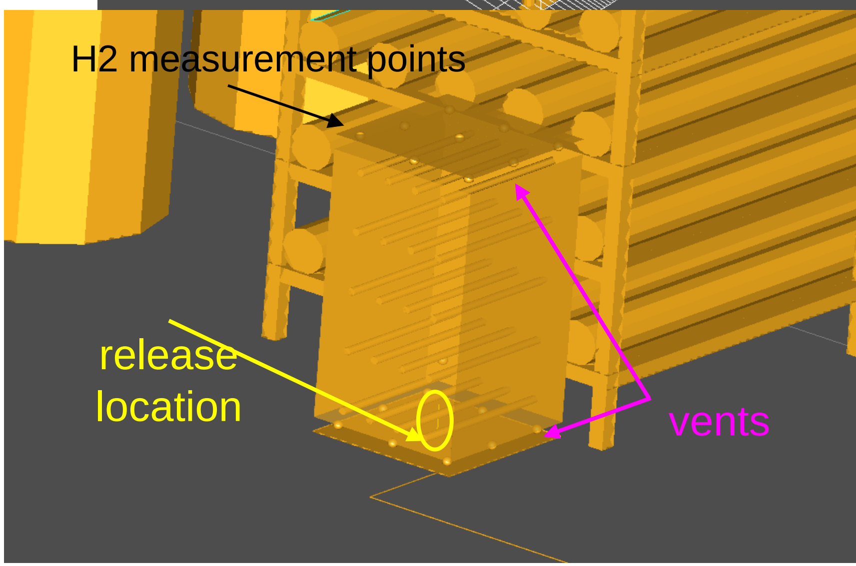
ADREA-HF applications

HySafe project: Hypothetical Hydrogen Refuelling Station

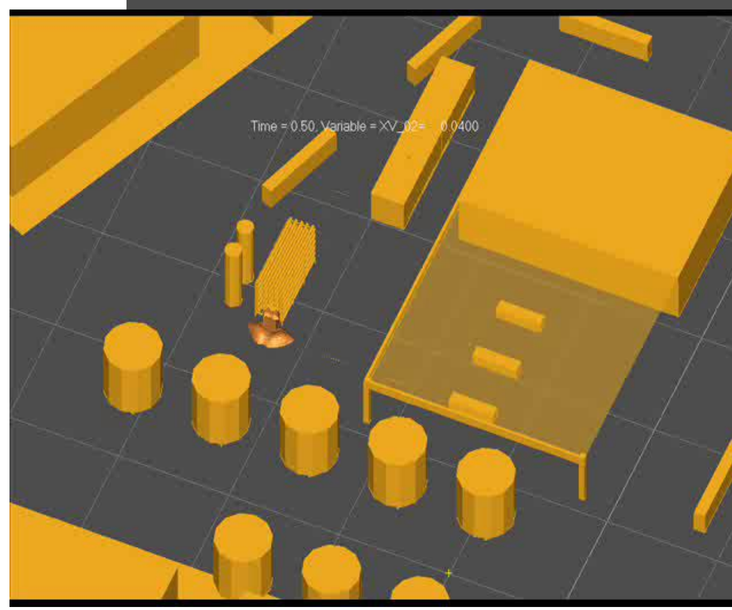
HyQRA







Scenario: Constant 1.2 Kg/s H_2 release (450 bar) for 5 s (ESD activation) dropping to zero in 20 s



See in Papanikolaou et al. (2011), Int. J. Hydrogen Energy, 36 (2011), pp. 2573-2581.

ADREA-HF code Links

www.demokritos.gr/erel

Venetsanos A.G., Papanikolaou E., Bartzis J.G.,

The ADREA-HF CFD code for consequence assessment of hydrogen applications,

Int. J. Hydrogen Energy 35 (2010) 3908–3918

Thank You