Research Priorities Workshop
BAM Berlin October 2012

Release and Dispersion Perspectives from GexCon, Norway

by

Prankul Middha

cmr Gexcon

Real life problems

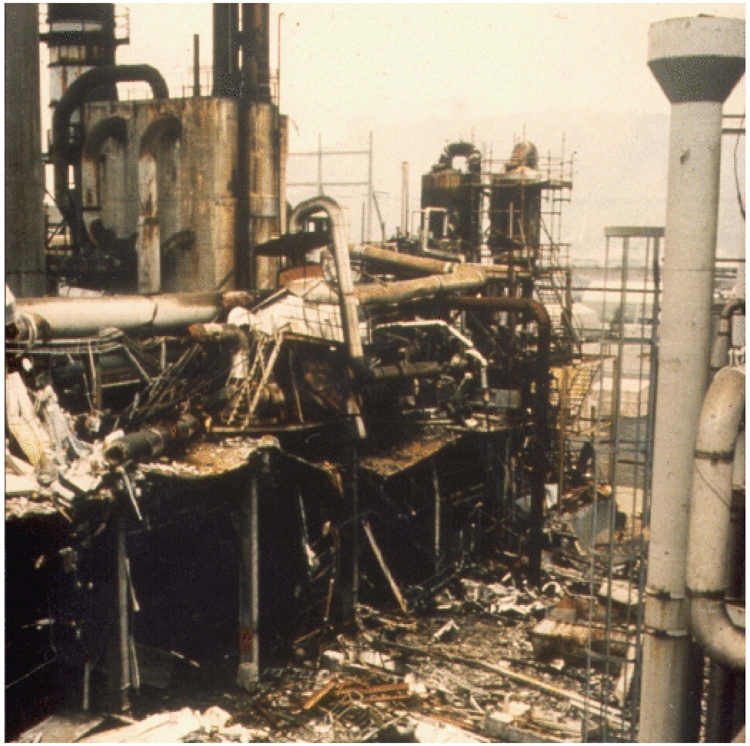
Which questions must be answered regarding hydrogen safety?

What is the risk, and how to minimize it, in connection to new H_2 infrastructure, transport, filling, production and storage?

What if there is a significant leak in a car, commercial vehicle or transport vehicle? What if inside tunnel or workshop?

How to prevent or minimize consequences of any internal explosion when starting to sell H_2 cars?

How to dimension a container or pipes with flammable H_2-air?

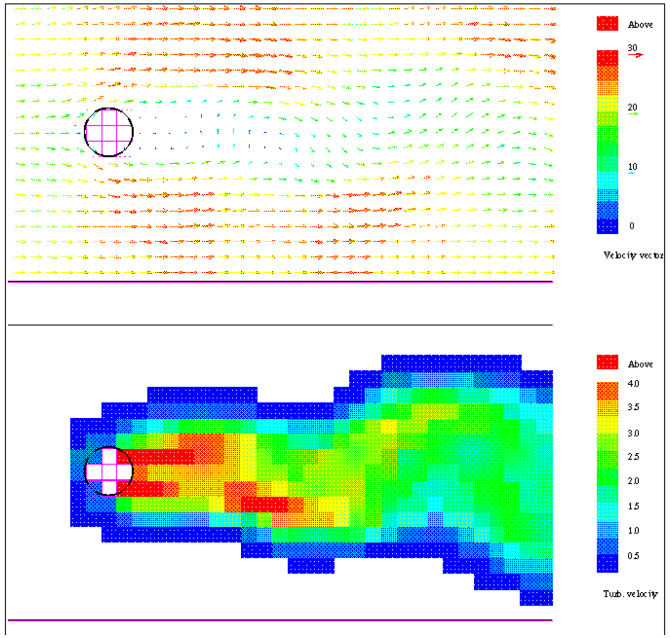


What if hydrogen leaks inside a congested process facility, e.g. chemical industry, nuclear facility or semi-conductor plant? How to design ventilation system in leak-exposed buildings? How to optimize wall strength and vents, and protect 3rd party neighbours?

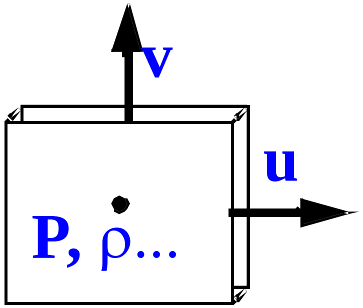
Will mitigation measures have a positive effect???

Methods available: CFD

CFD = Computational Fluid Dynamics



- Define a simulation domain (part of the real world)
- The domain is divided into boxes/volumes
- Define initial conditions and boundary conditions
- Solve conservation equations (Navier-Stokes + +)

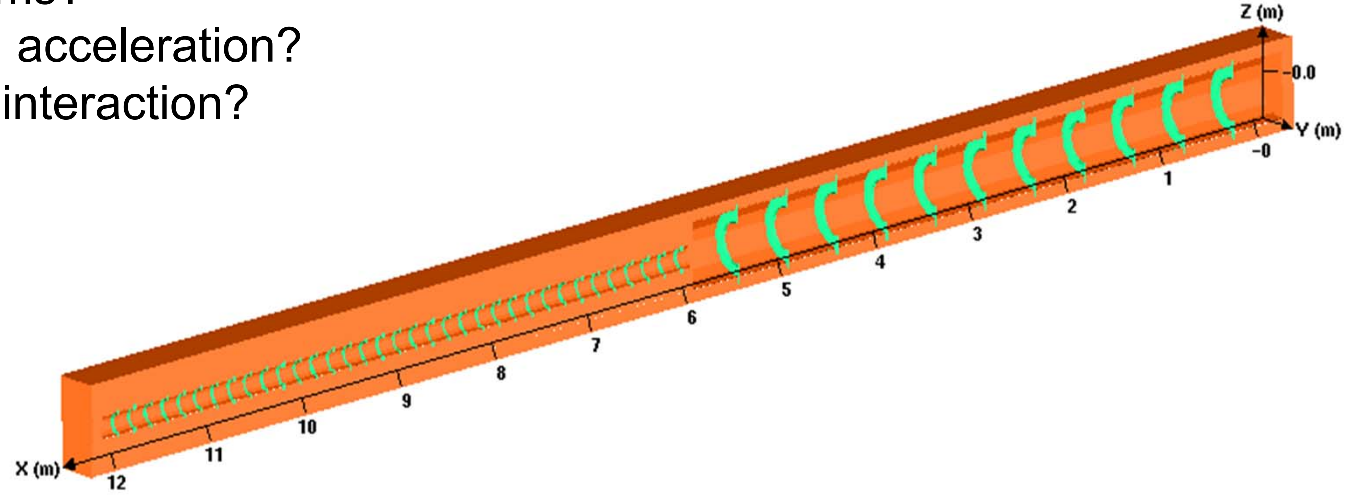


=> Predict what will happen in the real world

Methods available: Fundamental studies

Some issues being studied in scientific community:

- What are the flammability limits? What will influence them?
- Detonation flames, how to initiate and maintain?
- How many equations to include in reaction scheme?
- Ignition mechanisms?
- Flame stretch and acceleration?
- Turbulence flame interaction?

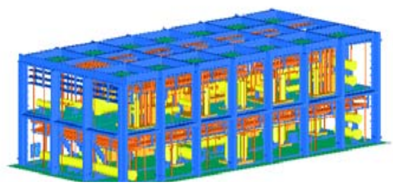


- **How can tests showing strong flame acceleration for 11% H_2 in an obstructed channel like this help to solve your real world problem?**

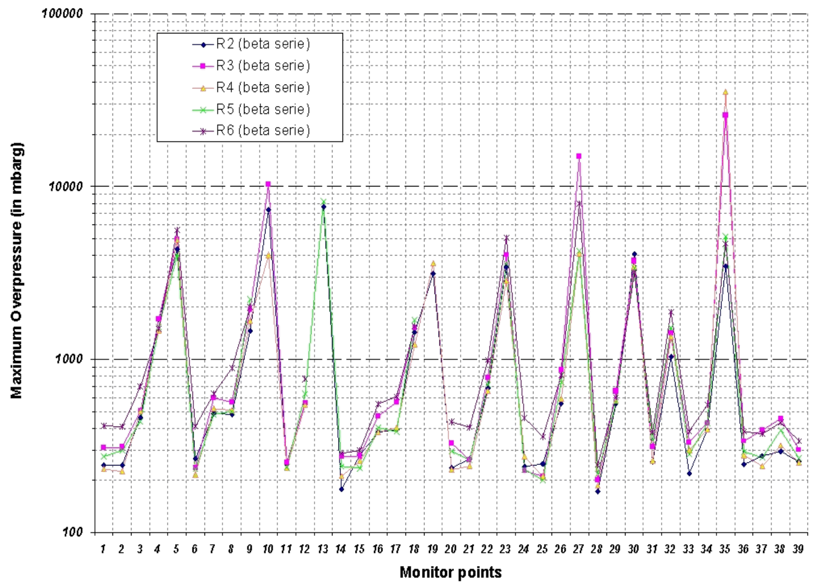
Your problem is seldom solved, but this input can be important when

- developing models
- evaluating model predictions

Methods available: Experiments?



- Experiments are expensive (prohibitive at full-scale?)
- Scale-down and simplifications of limited value
  - "Validation" of scaling often fails
  - Difficult to know impact of simplification
- Output from experiments usually limited
  - A few pressure-time histories
- Potential for errors
  - How is the repeatability?
  - Is measurement principle OK?



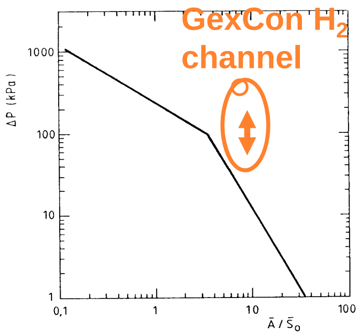
HSE/Advantica Phase 3A NG repeatability tests: Pressures in 5 "identical good quality repeats" varied by factor of 2 (low P) to factor of 10 (high P)

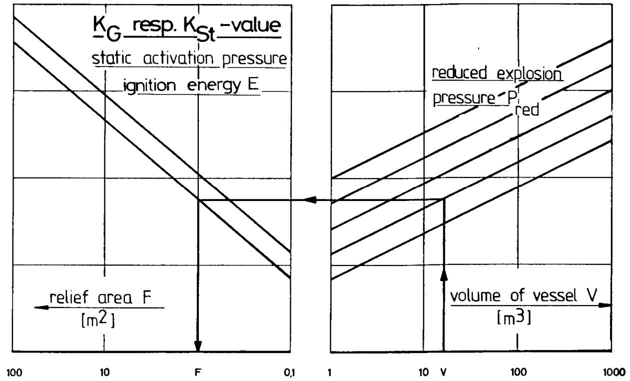
- Do the chosen tests answer the question asked?
  - Selected tests may be outliers or non-representative for hazard

Experiments alone seldom an optimal way to evaluate a potential risk!

Simplified methods useful?

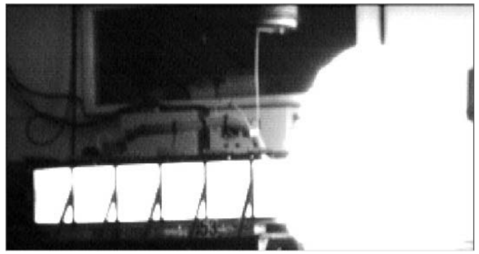
- Ventilation standards
  - Can gas clouds collect anywhere
- Explosion venting guidelines:
  - Use with care for realistic situations
- Far field blast loads:
  - Make sure these are conservative enough
- What about detonation?
  - Often too conservative to consider this





NFPA-68 (VDI3673): 0.52 barg
(0.83 barg with baffle at end)

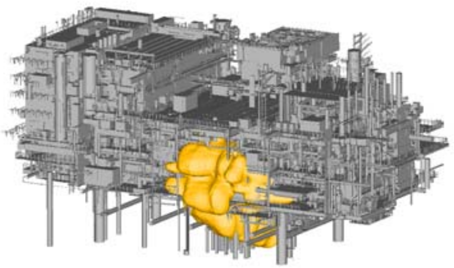
GexCon H_2 channel:
0.8 barg (empty)
1.7 barg (2 small baffles)
3.5 barg (4 small baffles)

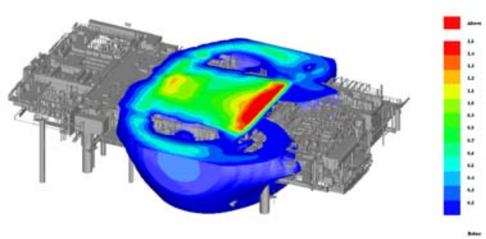


Simplified methods only use parts of the information available;
For a realistic situation they are sometimes not applicable (due to limitations).
If applicable, they may often be either non-conservative or far too conservative,
and can they tell the effect of a change or mitigation?

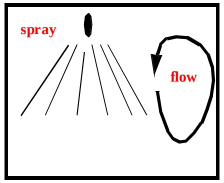
CFD could be the tool to combine knowledge

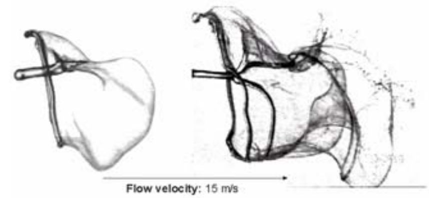
- Develop models based on
  - established equations
  - experimental input
  - fundamental studies
  - simplify where appropriate





- Many phenomena at smaller scales than realistic grid resolution (0.01m-1.00m)
  - flame reaction zone
  - obstructions
  - turbulence
  - water mitigation





1mm droplets break-up into μm mist to mitigate flames

Use dedicated experiments to develop sub-grid models

- DNS and detailed simulation approaches not so useful
  - Impossible to validate if each simulation will take weeks (or months)
  - Grid-dependent models will always remain (flame ++)

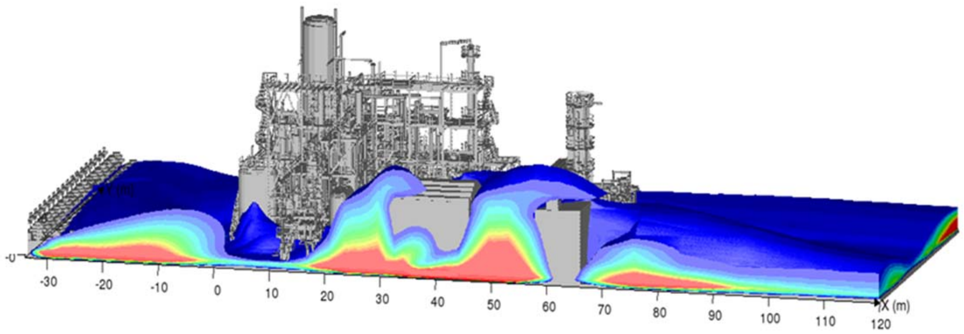
- Validate model by simulating 100s of tests

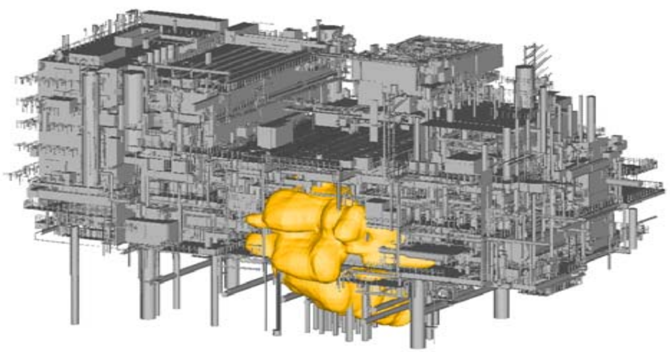
Both experiments, experts and simplified tools benefit from interaction with CFD (but also vice versa)

Release and Dispersion

CFD Software FLACS – Model Basics

- Specifically developed for **process safety** studies
- Full 3D Cartesian Navier-Stokes flow solver
- Distributed porosity concept – more efficient geometry handling
- Intelligent sub-grid models
- Validated against e.g. large-scale natural gas release and explosion experiments and LNG MEP database





Hydrogen Dispersion Validation in CFD tool FLACS

Basics from validation of FLACS for natural gas

- Ventilation
- Dispersion

Hydrogen specific validation

- Low momentum release (**Swain hallway**)
- Sub-sonic jets (**INERIS-6***, **Swain+**, **GexCon-D27+**, **CEA-Garage*, Shebeko***)
- High-pressure jets (**FZK+**, **INERIS+**, **HSL+**, ...)
- Impinging jets (**FZK-HySafe/InsHyde**)

* Slow diffusion also tested for INERIS-6, CEA-Garage and Shebeko

+ Horizontal releases; i.e. challenging as jets are deflected due to buoyancy

User independency

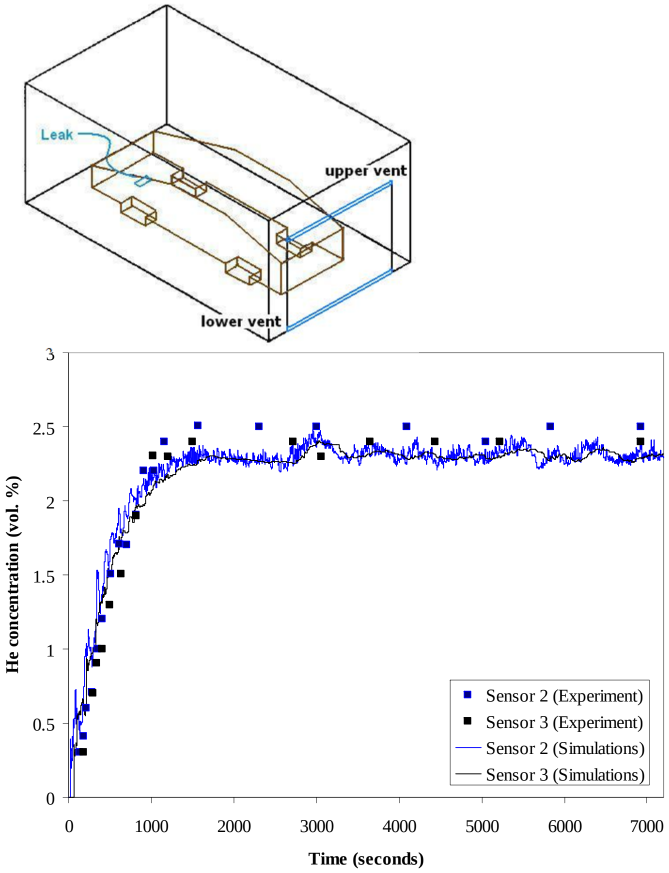
- INERIS-6 blind test
- Swain hallway (used as example at Hydrogen Summer School)

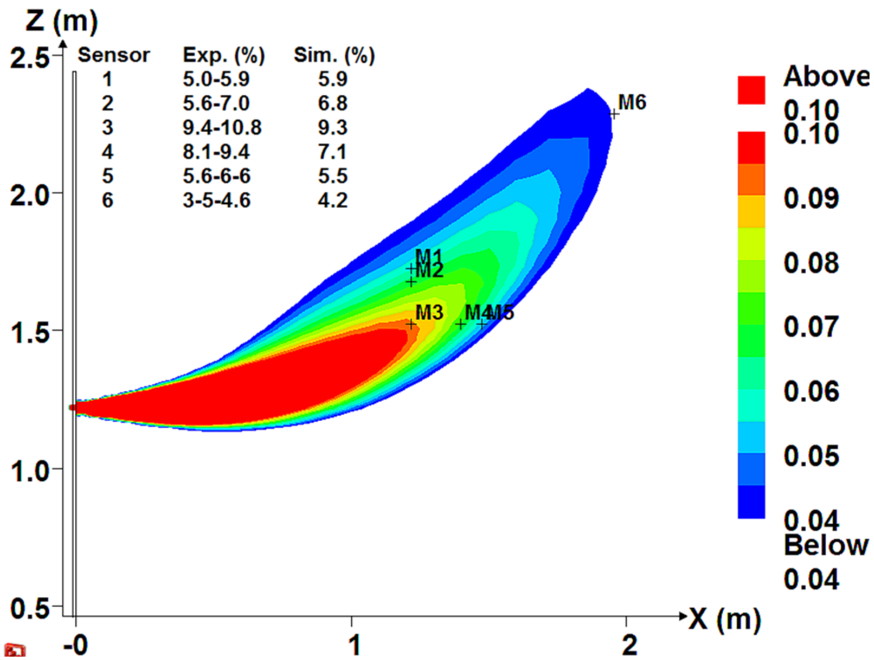
Models are also evaluated by others, e.g.

- Telemark University College against own experiments
- Hydrogen Research Institute / UQTR

Subsonic releases

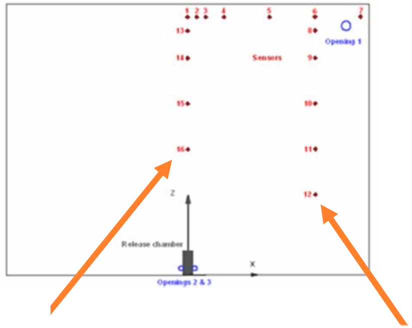
- Significant amount of work carried out
  - Benchmarks under HySafe
  - Other CFD studies and associated development
- Seems no major knowldge gaps in terms of prediction of scenarios
  - Simulations of oblique jets?

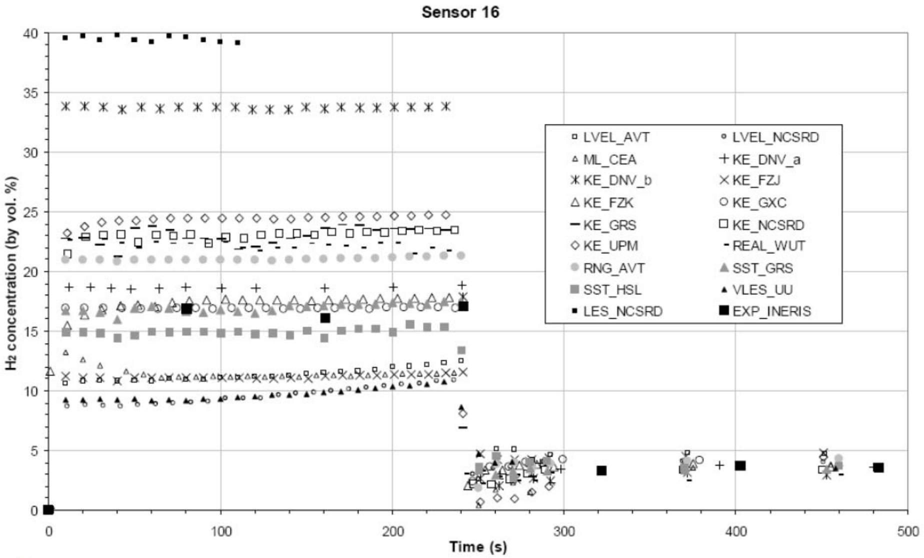


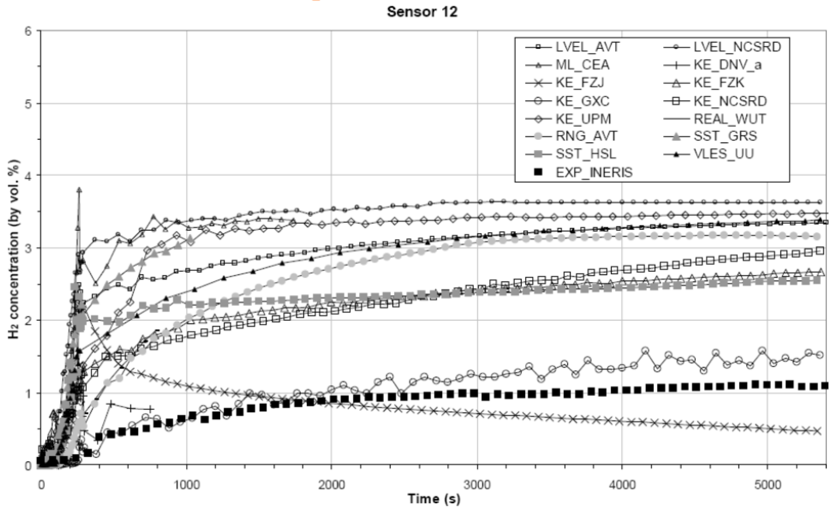


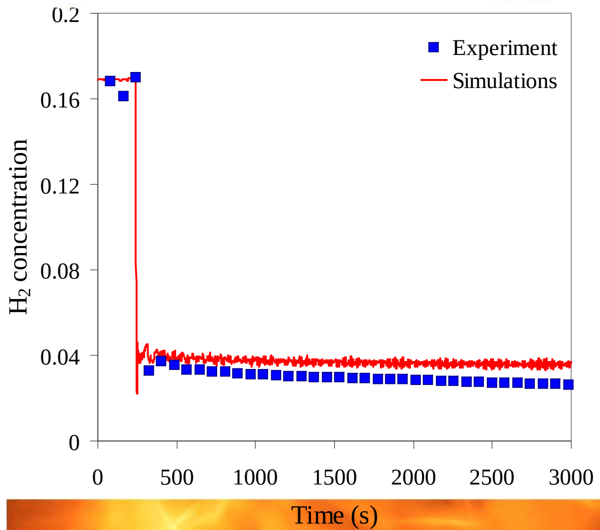
Note of caution

HySafe blind benchmark
From Venetsanos paper ICHS2/IJHE

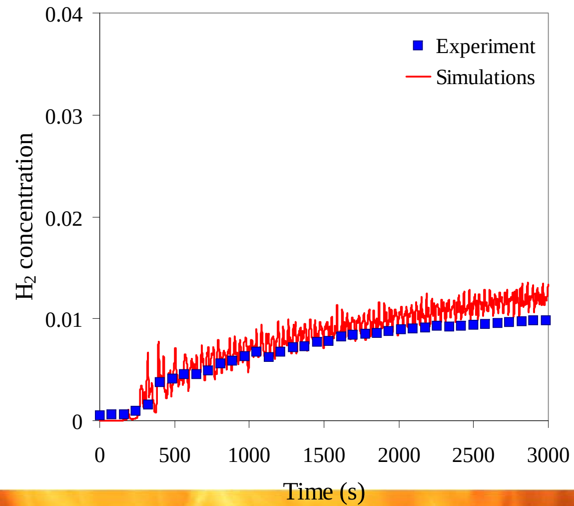






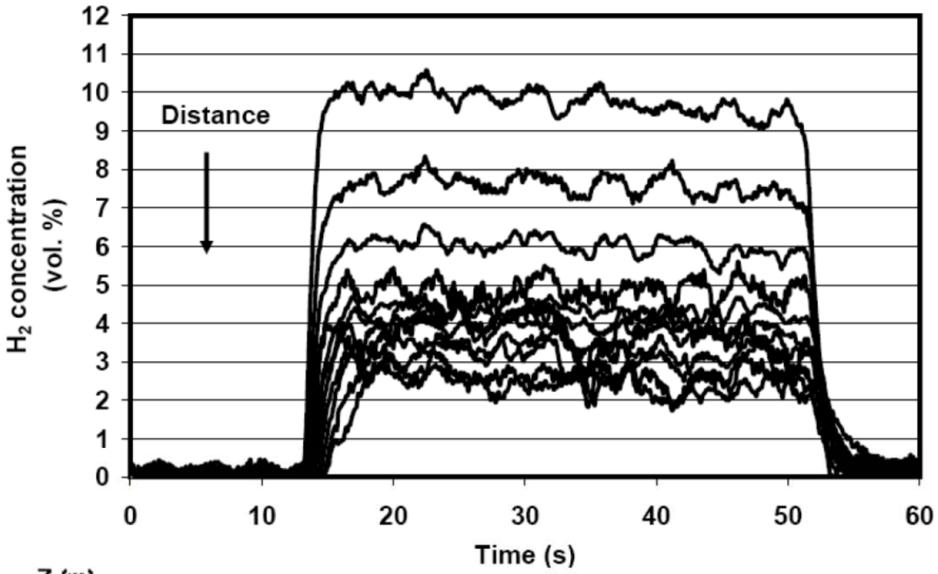


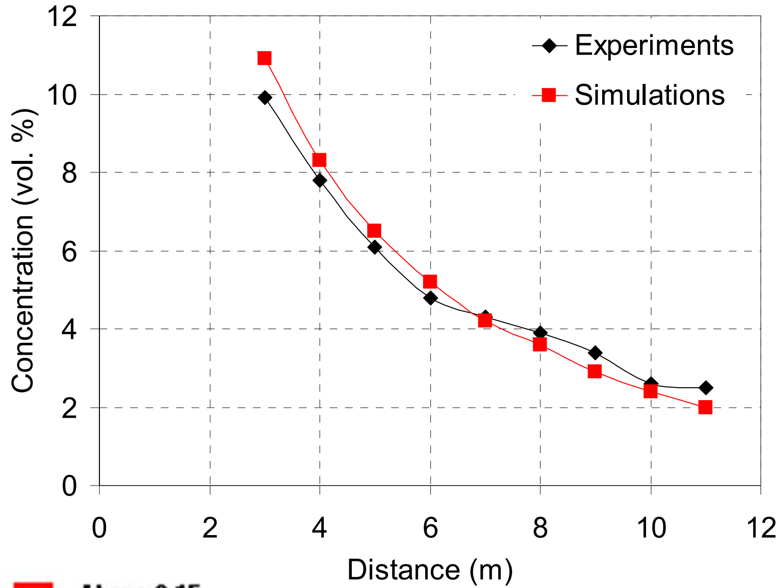
What is the status today?

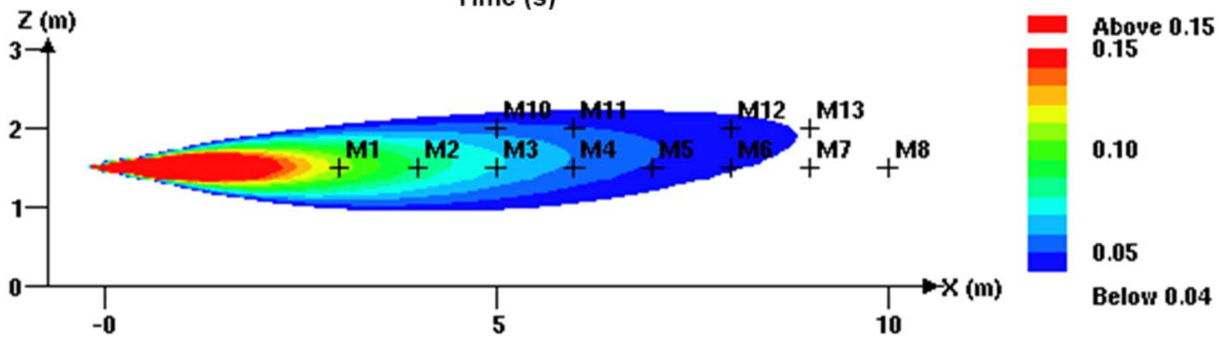


High pressure jets (HSL test 7)

- 100 bar release pressure, 3 mm nozzle (free jets)
- Strong effect of crosswind on concentration fields seen
- Good agreement with experimental data

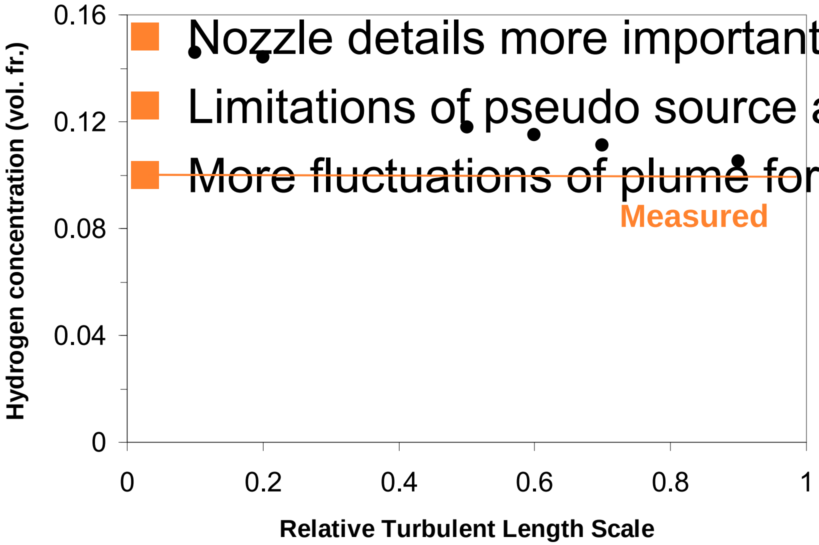




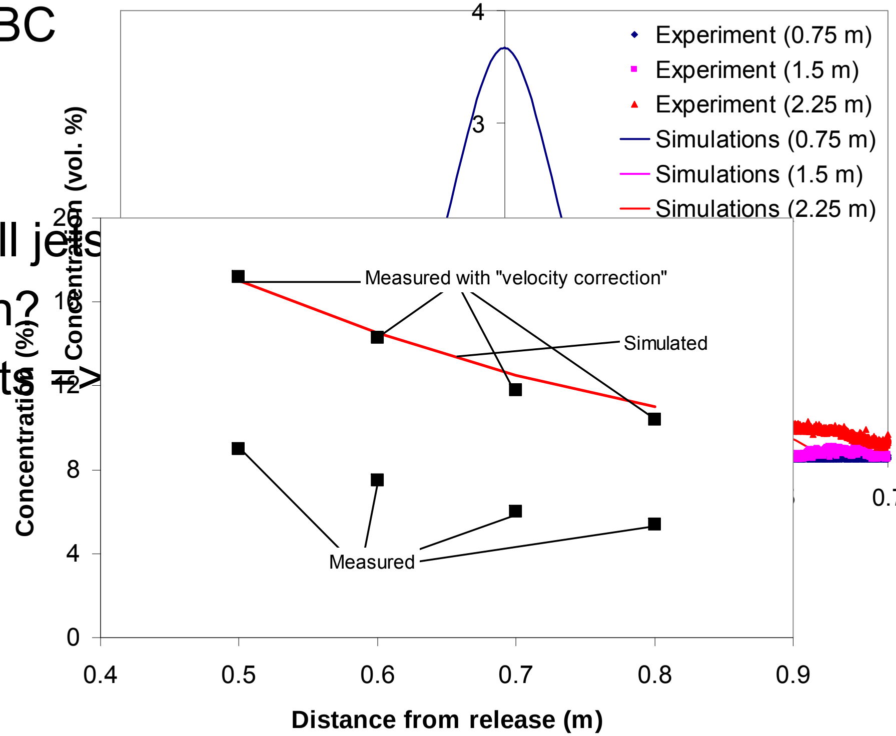


High pressure jets – INERIS & FZK

- Deviations seen when modelling INERIS jets (200 bar, 0.5 mm nozzle) and FZK jets (160 bar, 0.25 mm nozzle)
  - Experimental data overpredicted up to 2 times
- Attempts made to understand discrepancy
  - Variation of turbulence parameters in BC
  - Possible errors in oxygen sensors?
- Possible explanations to deviation:
  - Nozzle details more important for small jets
  - Limitations of pseudo source approach?
  - More fluctuations of plume for small jets



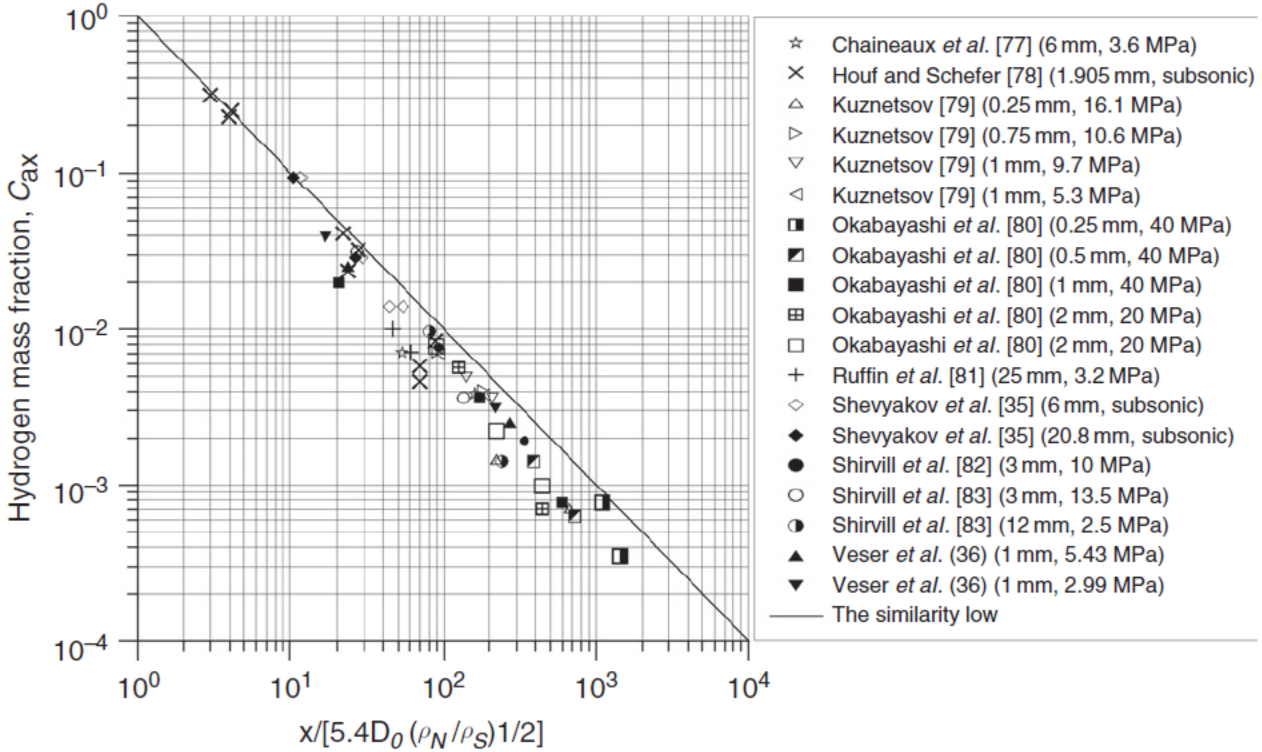
Concentration at 0.5m when RTI and TLS (relative to expanded jet dia) ↑ proportionally



Current Status

Significant work carried out in recent years on source term and underexpanded jets

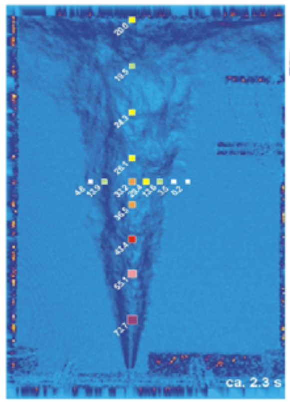
- E.g. Molkov and coworkers
- Efforts also on transition between momentum and bouyancy contolled jets

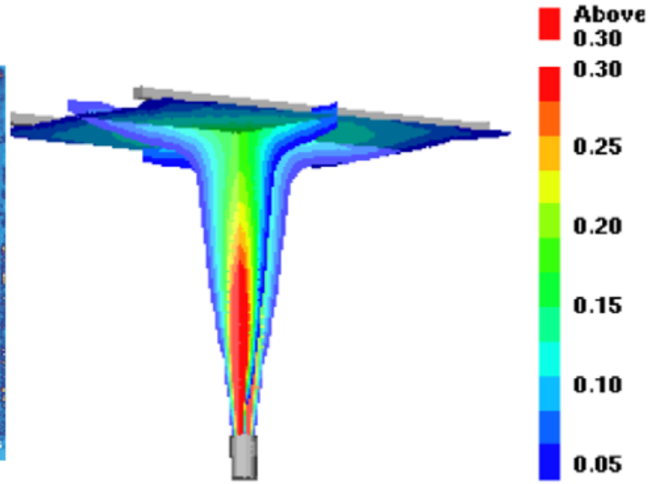


- Able-Noble equation added in CFD tool(s) for more accurate simulations at high pressures
- However still unclear whether all issues described in previous slide are handled completely?
  - Work with Venetsanos, Baraldi and coworkers with 4-5 notional nozzle models, 3 turbulence models also shows performance deteriorates with decreasing nozzle dia

What else is missing?

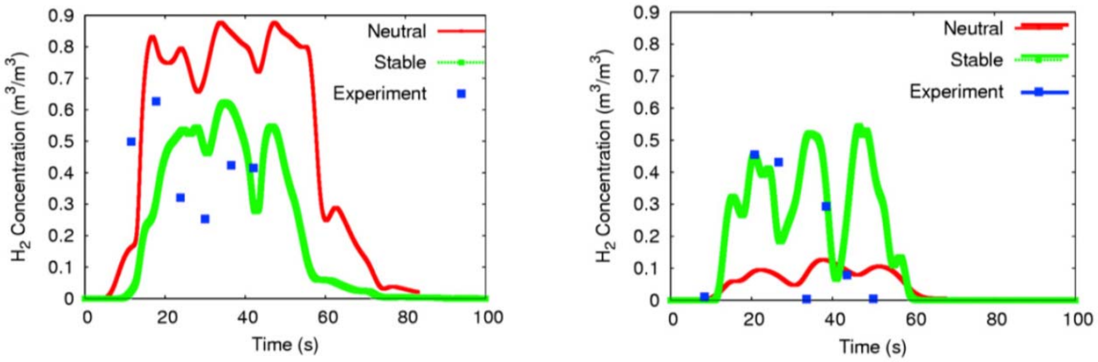
- Still only limited validation of simulation studies in real complex configurations such as with obstacles, barriers, etc.
  - Sandia Barrier experiments
  - FZK impinging jets
- Surface effects?
  - Simulation studies by HRI/UQTR
  - Proposal on experimental validation
- Effect of natural & forced ventilation
  - Vent configurations
  - Wind in outdoor releases in complex geometries
    - Some work by Carcassi & coworkers recently but only in “empty” geometry





LH_2 releases - simulations

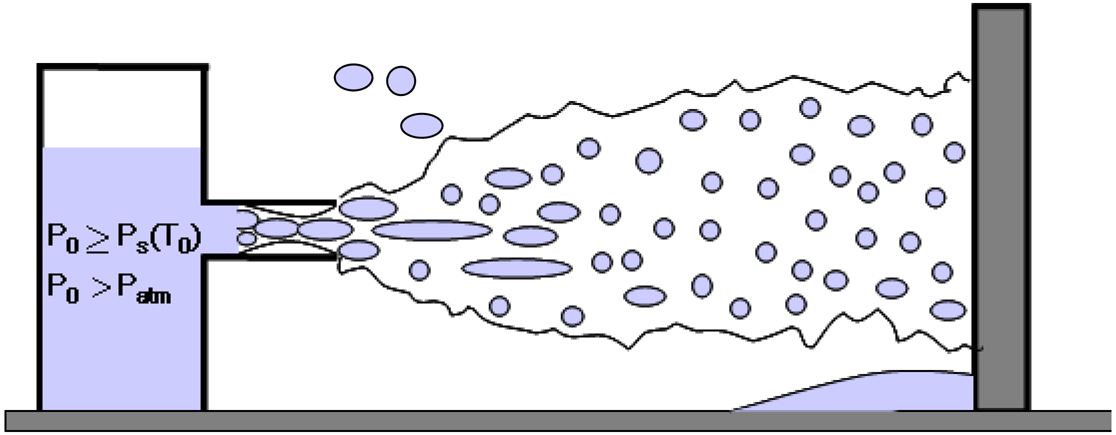
- The BAM experiments
  - LH_2 releases between buildings (0.37 kg/s; duration 125 s)
- The NASA experiments
  - LH_2 releases on flat terrain (11.5 kg/s; duration 35 s)



- Significant efforts in LNG related work
  - Burro, Coyote, Maplin Sands and Wind tunnel experiments simulated (MEP – Hansen et al., 2010)

Multiphase flow modelling in FLACS

- Homogeneous Equilibrium Model (HEM) used for modeling two-phase flows
- Both phases assumed to be in local thermal and kinematic equilibrium
- Model for liquid deposition on obstacles



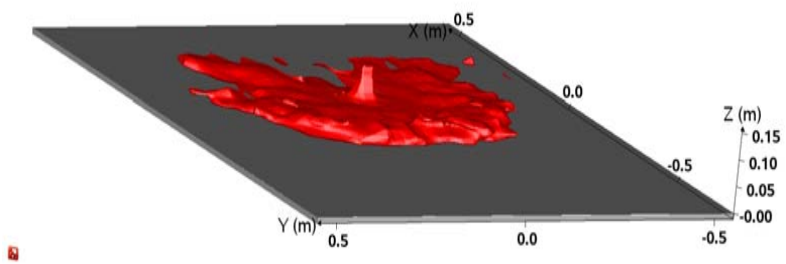
- Rain-out due to jet impingement on obstacles: rain-out is controlled by the momentum of the jet; Mass of liquid that rains out directly transferred to the pool model

HSL experiments

- The HSL experiments (4 tests in total):
  - 2 vertically downward releases 100 mm above ground (Tests 6 and 10)
  - 1 horizontal release 860 mm above ground (Test 7)
  - 1 horizontal release on the ground (Test 5)
  - Release rate: 60 l/min

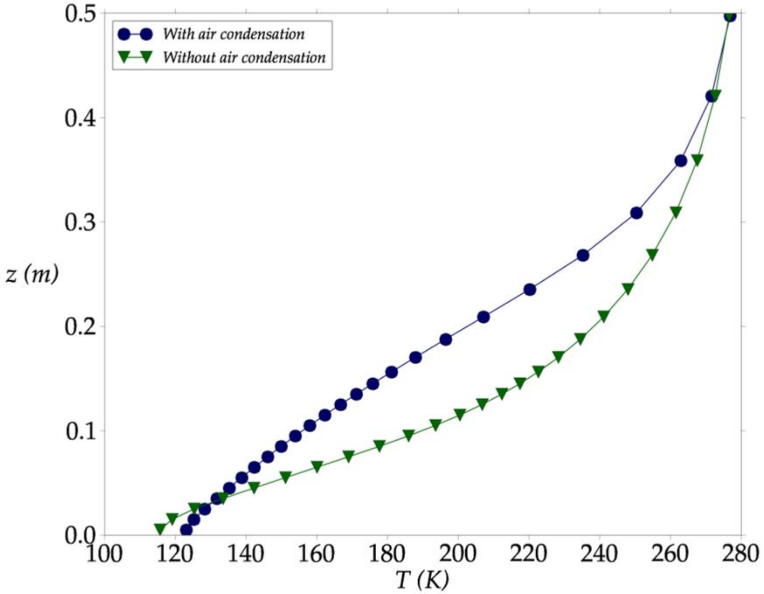
Simulations of HSL experiments

- Simulation of Test 6 with ST4:
  - Downward release 100 mm above the ground
  - Investigate the effect of air condensation.
  - Boiling point of O_2 is 90K and N_2 is 77 K
  - Volume contour plot of temperature at T=77 K: condensing/freezing zone of N_2 and O_2

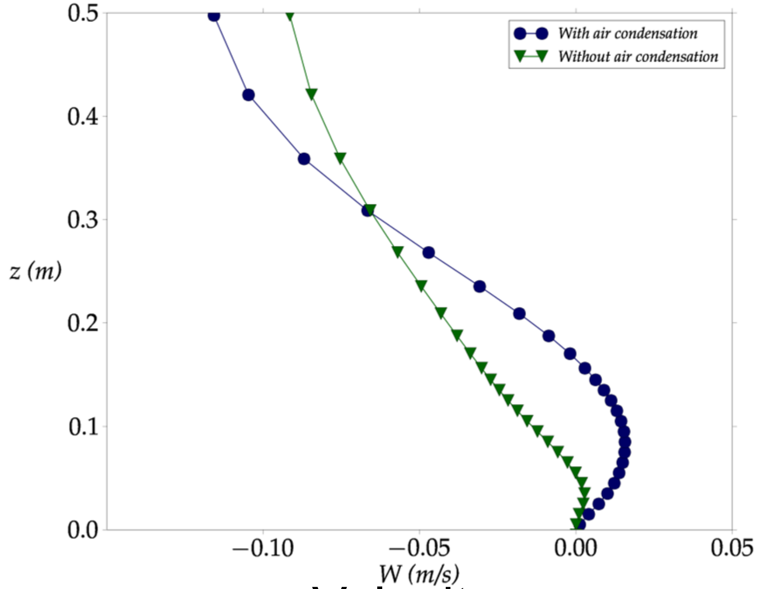


Simulations of HSL experiments

- Effect of air condensation (Test 6)



Temperature



Velocity

Vertical profiles 1.5 m downstream of exit orifice

LH_2 knowledge gaps

- Prediction capability OK
  - Condensation of O_2 and N_2 can have non-negligible effects on the flow field
  - Condensation of water vapor may also have non-negligible effects
- Effect of wind and atmospheric conditions?
- More LH_2 spill tests should be performed (Evaluation protocol like for LNG?)
  - Potentially a very hazardous scenario, on hot summer days, LH_2 vapour may stay dense!
  - Mixed with air to stoichiometric concentration => -60ºC
  - At this temperature H_2-air mixture contains ~30% more energy => potential for very severe explosions
  - Evaluate explosion of cold H_2-air mixtures + vegetation/objects

Risk assessment

- Lot of efforts (e.g LaChance) on leak frequencies
  - Still need for more data to close the gap with O&G

- Existing approaches for cloud and ignition parameters
  - Ignition time
    - Time of max flammable mass/volume
    - Time of max equivalent stoichiometric cloud volume
  - Which cloud to ignite
    - The real cloud
    - The equivalent stoichiometric cloud
      - Where to place this equivalent cloud
  - At which position to ignite
  - Effect of jet turbulence when igniting releases?
  - Is turbulence behaviour different depending on release pressure?

- Suggestion for future work
  - Systematically evaluate and inter-compare existing approaches

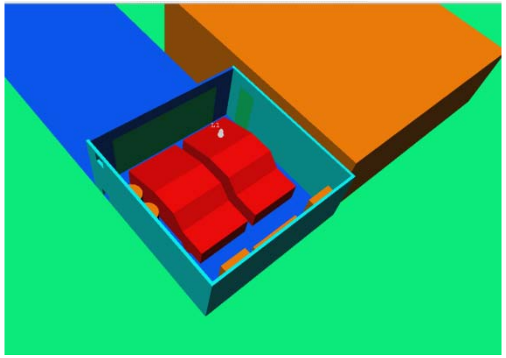
How about hydrogen/methane mixtures?

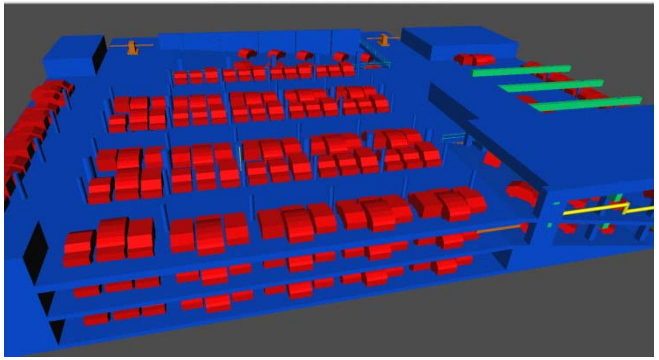
How is Hythane safety relative to CH_4? Can buoyancy compensate higher reactivity?

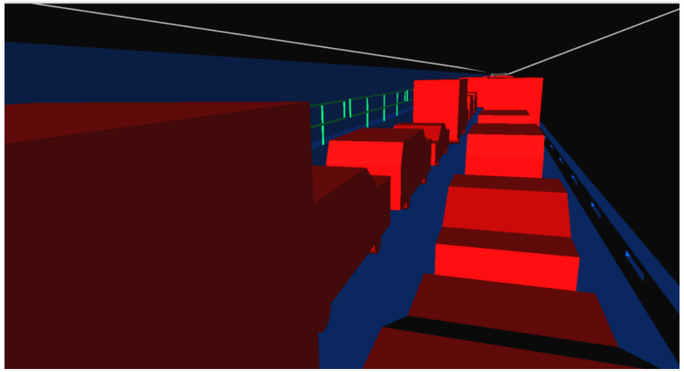
Approach:

Perform simulation studies of various situations and compare “realistic worst-case” explosions:

- PRD release from car in private garage
- PRD release from car in public parking garage (narrow corner versus more open location)
- PRD release from bus in narrow tunnel (cross-section 25m^2)







Definitions	
Worst-case	Full volume or all released gas with WC ignition locations
Realistic worst-case	**Most hazardous cloud from dispersion ignited at WC location**
Probabilitistic	Pressure exceedance curve based on 100s of disp+ign cases

Results

FLACS used to study Hythane safety, as compared to methane and hydrogen

- Some validation simulations were performed with good results (Shell/HSL tests)

- Private garage; gas may accumulate (even with much lower release rates than studied)
  H_2 >> hythane > CH_4 **House may survive CH_4 and hythane, H_2 more questionable**
- In parking garages local geometry layout will define hazards
  Narrow spaces (low ceiling & corners) may be a problem with H_2, other places not
  H_2 >> hythane > CH_4 (car in parking garage) **Mainly H_2 in narrow places concern?**
- In narrow 2 lane unidirectional congested tunnels (typical e.g. for US cities)
  H_2 > CH_4 > hythane (Bus in tunnel) **All cases of concern, and Hythane > CH_4**

Could not demonstrate Hythane to be safer than methane, but comparable

Please notice:

We have been studying worst-case scenarios only.

Non-ignited PRD releases may not be credible events => study may be far too conservative

Final words

- Still some efforts needed in release and dispersion for hydrogen safety
- Knowledge gap discussion should focus on major uncertainties in quantitative risk assessment.
- Knowledge gaps ignored e.g. in oil and gas industry does not necessarily have to be removed before calculating risk for hydrogen.
- Frequencies and probabilities for leaks and different ignition mechanisms will have significant uncertainties if a probabilistic QRA approach shall be developed. To estimate and model good assumptions for these would be of importance.