Experiences obtained in the course of HySafe project

ADVANCES IN MODELING FOR SAFETY APPLICATIONS

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Motivation

Mostly damages in industrial accidents are resulted from explosions of combustible gases … and among other combustible gases H_2 has unique properties, which makes it one of the most dangerous agent

Thus we are going to speak here about numerical modeling of possible accidents in industry with H_2

What are the tasks for CFD in safety: there is a need in better understanding and in development of complete modeling procedure with the view:

- to predict accident progress and consequences
- to develop efficient mitigation measures
- to provide reliable data base for rules, codes and standards
- to support development of safe hydrogen technologies

How to fulfill these tasks ?

How to fulfill the tasks ?

How to realize all these missions numerically to obtain physically rational result ?

There are exists a number of physical and numerical models with approved quality …

… but mostly the such models are too demanding to computer power and they require resolution not achievable in practical cases. Thus modelers often are not so deliberate in the choice of models and resolutions.

One of the way to provide the quality of engineering simulations is to test against existing full scale experimental data …

and as a result of such testing to select the models usable for practical simulations (time and grid size).

In the frames of EC project HySafe a benchmarking curriculum was established with the aim to provide progress in the area of CFD simulations for hydrogen application safety

CFD benchmarking activity in HySafe

- Partners prepared benchmark experimental database which includes 33 experiments from literature and from project partners
- During period from 2004 – 2009 calculation teams from 13 project organizations performed simulation of 21 experiments
- 9 simulations were chosen with the focus on dispersion and 12 simulations on deflagration

- Series of calculations was performed in support of the internal projects as InsHyDe (confined explosions) and HyTunnel (auto tunnels), etc. They included pre-test simulations for verification of the installation set-ups and post-test simulation for complement analysis of the experimental data
- Series of calculations in support of the external EU projects as HyApproval (H_2 refueling station), HyPER (H_2 stationary applications), etc

- 14 meetings for simulation discussions; ≈ 3 meetings / year
- 11 publications (only common papers)

Scenario, phenomena and models

Scenario

- Source
- Mixture formation
- Ignition
- Combustion
- Consequences

Phenomena classes

- Gaseous leak
- Liquid leak
- Dispersion of gaseous cloud
- Ignition
- Gaseous combustion
- Spill combustion

Individual phenomena

- Laminar flame
- Flame acceleration / deceleration
- Turbulent deflagration
- DDT
- Detonation
- Quenching
- Fire

Physical and numerical models

- Gas-dynamics (NS, instationary, compressible, single phase, ...)
- Thermodynamic properties of gases (H2, N2, O2, …)
- Turbulence
- Chemical kinetics / Turbulent combustion model including quench
- Heat transfer / Radiation

Priority directions in SBEP modeling

Dispersion program

- Single phenomena oriented
  - Dispersion in single-compartment
  - Dispersion in multi-compartment environment
  - Jet modeling
- Application oriented
  - Garage environment
  - Tunnel environment

Partners expert selection

Input from Phenomena Identification and Ranking Technique (PIRT) analysis for 166 possible accidental events in H_2 applications

Deflagration program

- Single phenomena oriented
  - Unconfined deflagration in the open area
  - Single-compartment, non-uniform mixtures
  - Jet
  - Vented deflagration
  - DDT and detonation
- Application oriented
  - Refueling station environment
  - Tunnel environment

Factors influencing the severity of the accident

- Jets
- Convection & Ventilation
- Confinement & Obstruction
- Scale

→

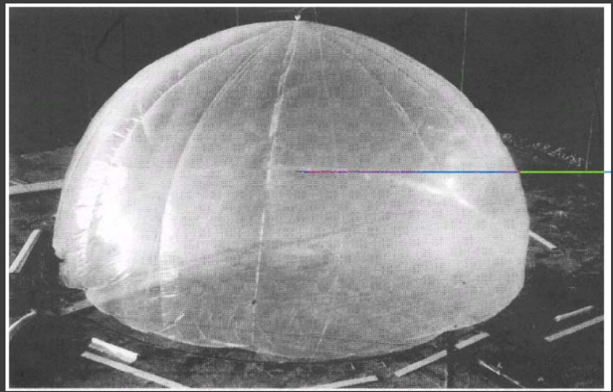
- Fast flames
- Flame acceleration
- DDT
- Detonation

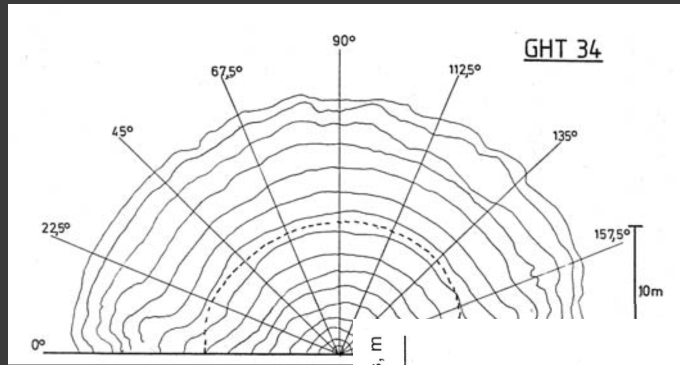
Dispersion benchmarks	Phenomena / Environmental Conditions						
	Low momentum jets	Sonic jets	Confinement	Vertical Diffusion	Forced Ventilation	Natural ventilation	Obstacles
SBEP-V1	√		√	√			
SBEP-V3	√		√	√			
SBEP-V4		√					
SBEP-V5	√		√			√	√
SBEP-V6				√		√	
SBEP-V10		√					
SBEP-V11	√		√	√		√	√
SBEP-V20	√		√	√		√	√
SBEP-V21	√		√	√		√	√

Combustion and explosion benchmarks	Phenomena / Environmental Conditions						
	Unconfined combustion	Partial confinement/ Venting	Complete confinement	Slow flames	Fast flames Flame acceleration	DDT Detonation	Scale
SBEP-V2	√			√			√
SBEP-V7	√			√			√
SBEP-V8		√			√		
SBEP-V9		√			√	√	√
SBEP-V12		√			√		√
SBEP-V13		√	√			√	√
SBEP-V14		√		√	√		
SBEP-V15		√		√	√		√
SBEP-V16		√		√	√		
SBEP-V17		√			√		
SBEP-V18			√	√			
SBEP-V19		√	√		√	√	√

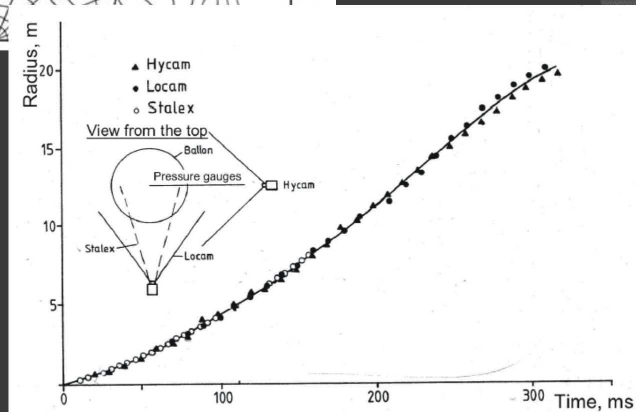
Phenomena oriented simulations

Large-scale deflagrations in open surroundings





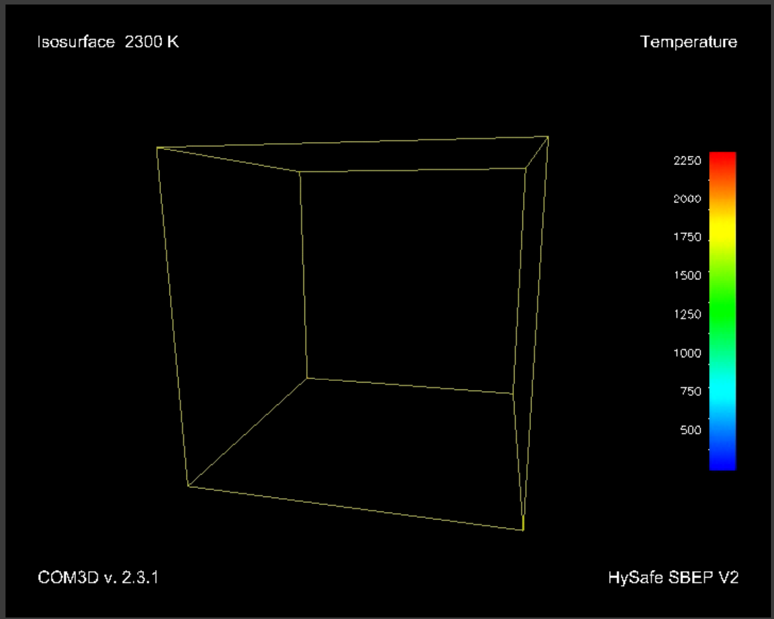
SBEP V2

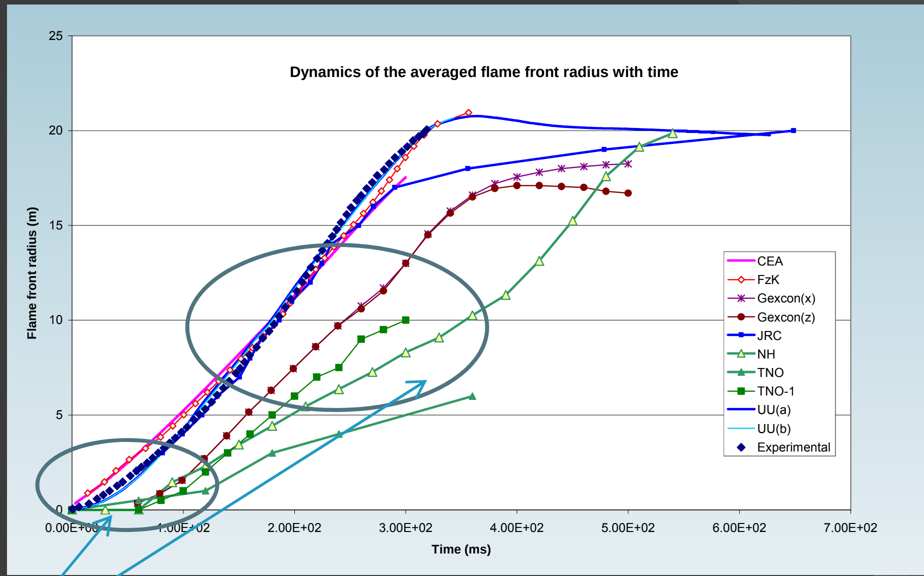


Combustion of 10 m radius hemisphere
with 30% hydrogen-air mixture

7 partners
Resolution: 0.1 – 1 m and adaptive
Turbulence: algebraic – RANS – LES
Combustion: various (Adjusted speed - EDM - St(U´))

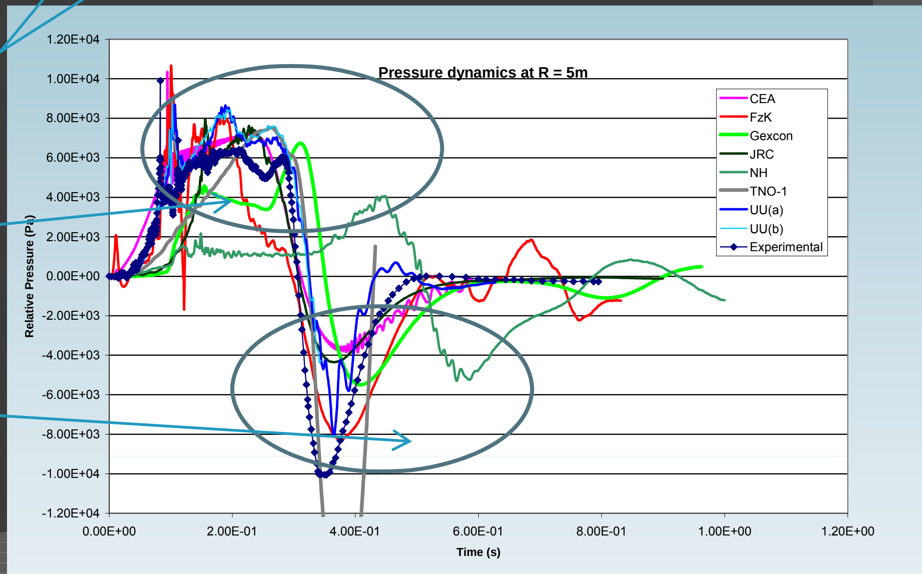
Address:
Deflagration development dynamics in open atmosphere
with resulting pressure wave generation





Success:
- Correct deflagration speed
- Positive phase of pressure wave

Problem:
- Initial flame acceleration
- Negative phase of pressure wave



Subsonic horizontal jet release in a multi-compartment room

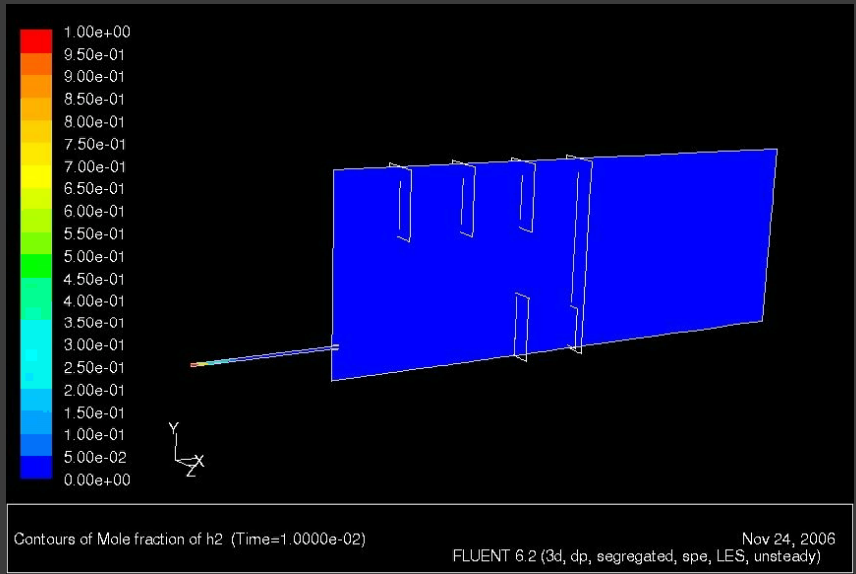
SBEP V5

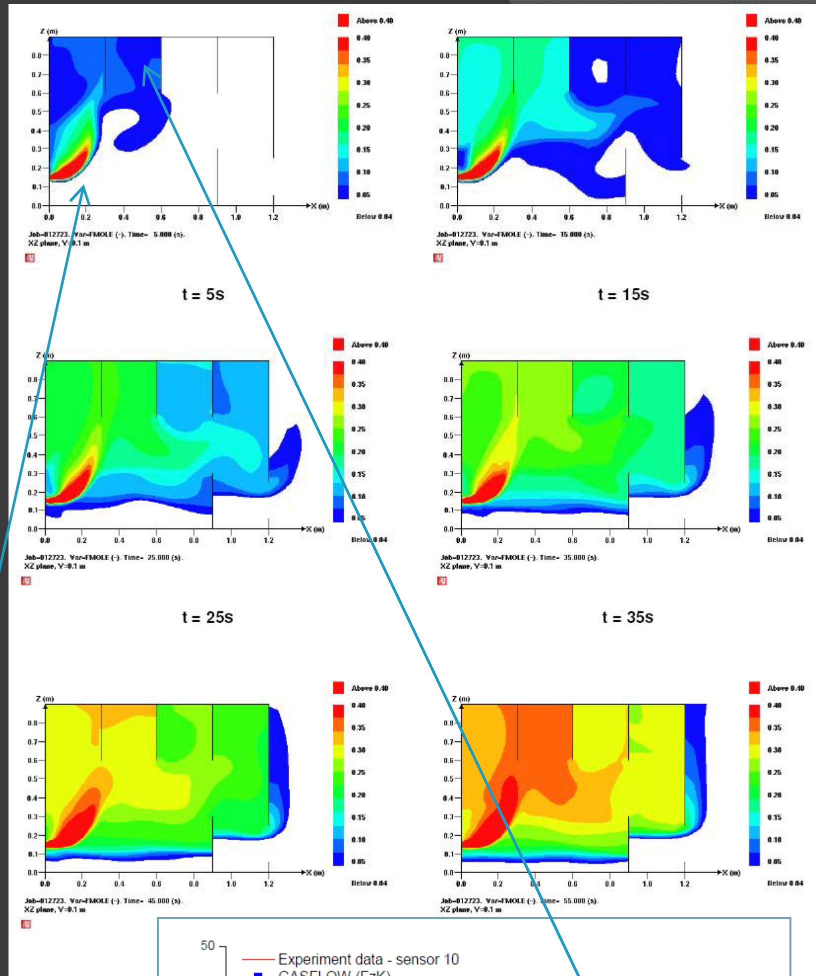
The experimental rig 1.20 m × 0.20 m × 0.90 m, with compartments 0.30 m × 0.20 m

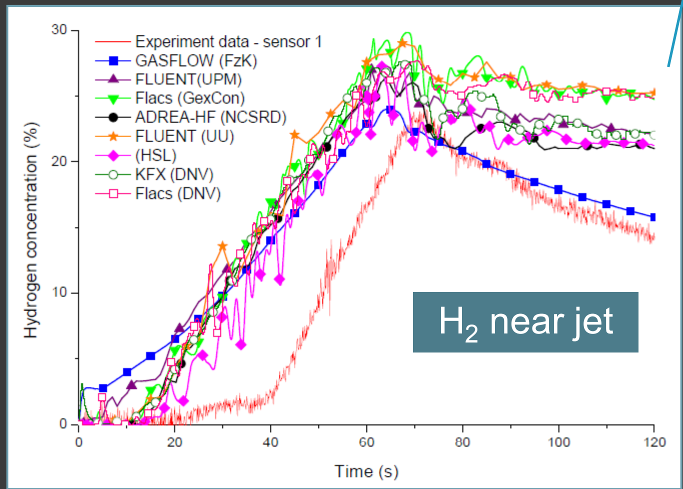
Release time, s	Nozzle diameter , mm	Exit velocity , m/s	Flow rate, Nl/s	Xjet, m	Yjet, m	Zjet, m
60	12	10.17	1.15	0.03	0.1	0.145

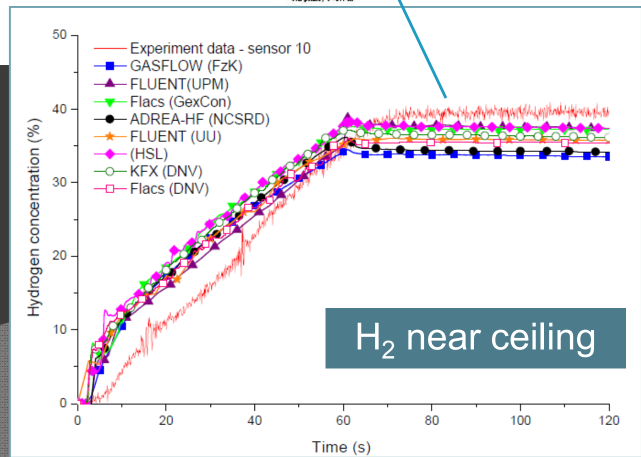
Address:
Dispersion phenomena implied with a low momentum horizontal hydrogen jet release in a multi-compartment room

6 partners
Resolution: variable 0.005 – 0.30 m (23 000 – 260 000)
Turbulence: RANS – LES







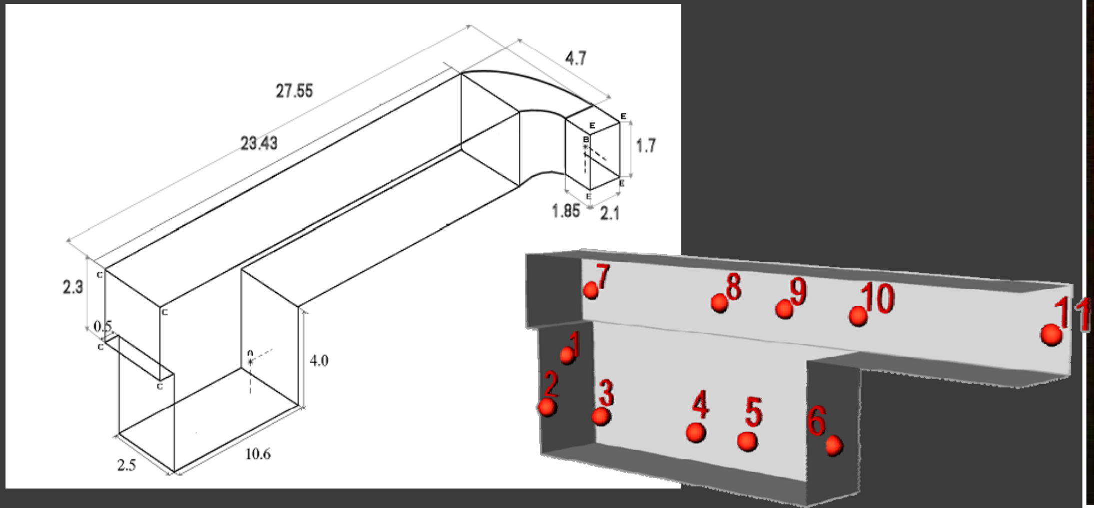


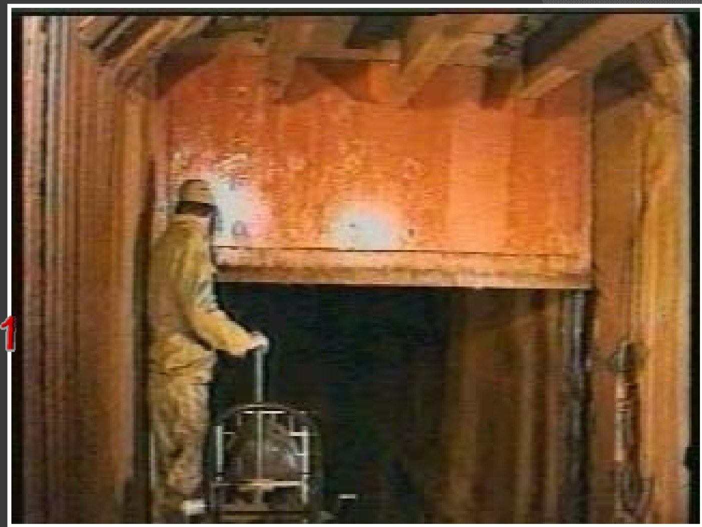
Satisfactory predicts stratification and growing time for upper gauges and near exit

Fail to predict jet entrance area

Detonation in large scale

SBEP V13

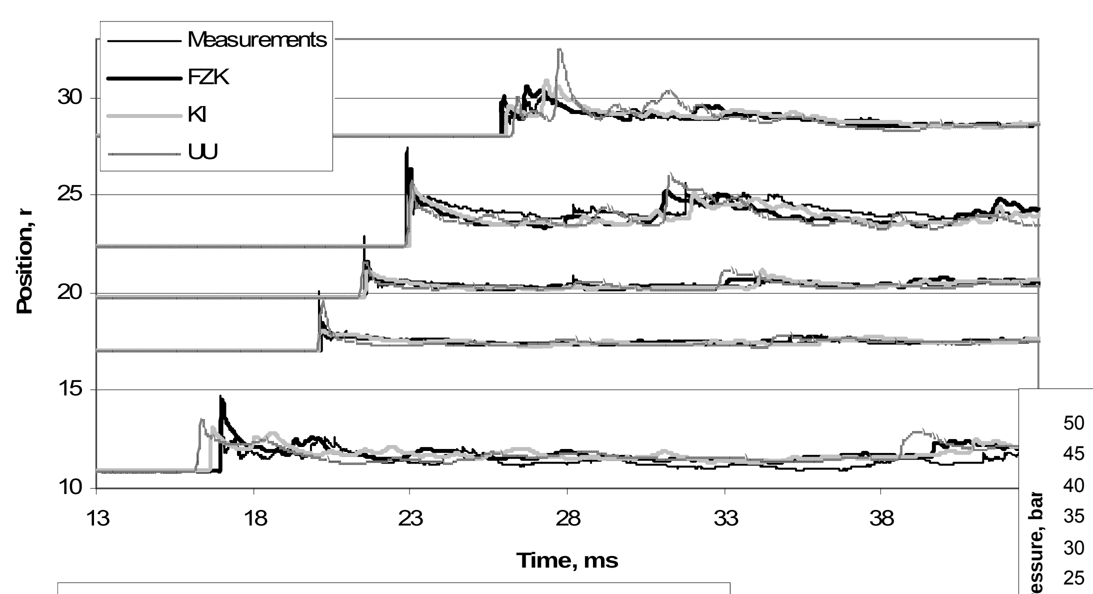




Detonation experiments in large scale confined complex geometry
28 x 7 x 2.5 m -> 263 m^3
Uniform hydrogen/air mixture with concentration of
20.0% and 25.5% H_2 in air

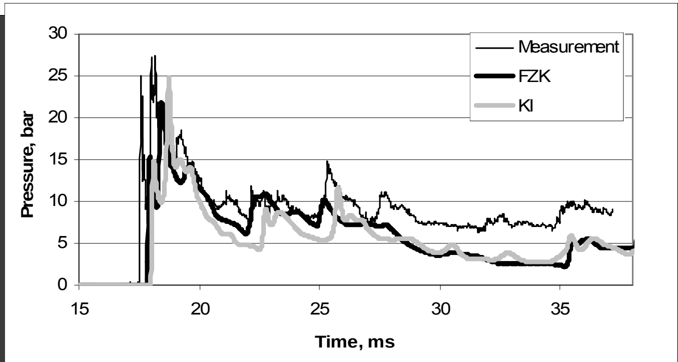
Detonation wave propagation and pressure loads in the complex geometry.
Challenging experiments for the codes validation on detonation simulations on scales relevant to industrial
Only 3 partner took part

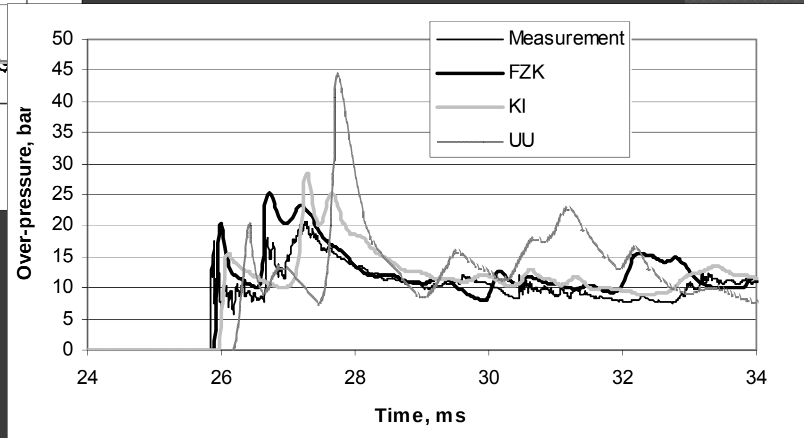
W. Breitung, S.B. Dorofeev, A.A. Efimenko, A.S. Kotchourko, R. Redlinger, V.P. Sidorov.
Proc. 20th Int. Symp. on Shock Waves, Pasadena, CA, USA, 1995, p. 405



Resolution: 6.7 cm and 10 cm
Solvers:
1-order and 2 order upwind
Chemical interaction models:

- 1-step Arrhenius
- Artificial detonation
- Gradient combustion





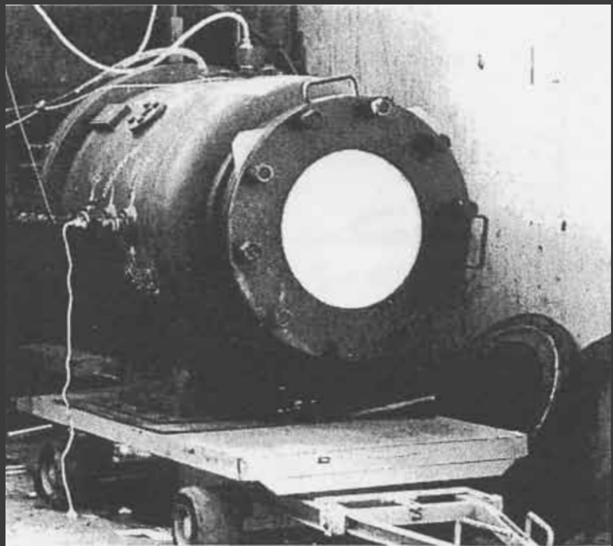
In the areas of steady state detonation even on the coarse grids (calculation cell size of ~ 6-10 cm >> detonation cell size ~ 1.2 to 2.2 cm) the quantitative results are very good for the propagation speeds, overpressures and impulses

Not all models have the same quality for different concentrations

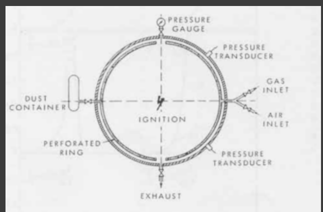
The main outcome is that the simulation of detonations in large scale can be considered as reliable and trustworthy

H_2-air vented explosion

SBEP V14



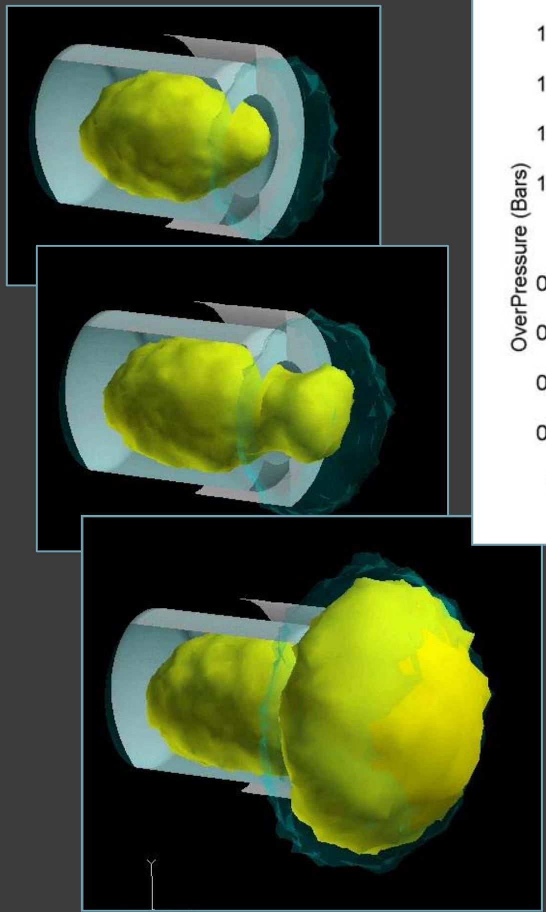
- 29.6 % H_2-air mixture
- $1.018.10^5$ Pa, 281 K
- ~0.95 m^3
- Centered ignition
- Three test configuration
  - Closed
  - Open 0.3 m^2 with rupture membrane
  - Open 0.2 m^2 with rupture membrane

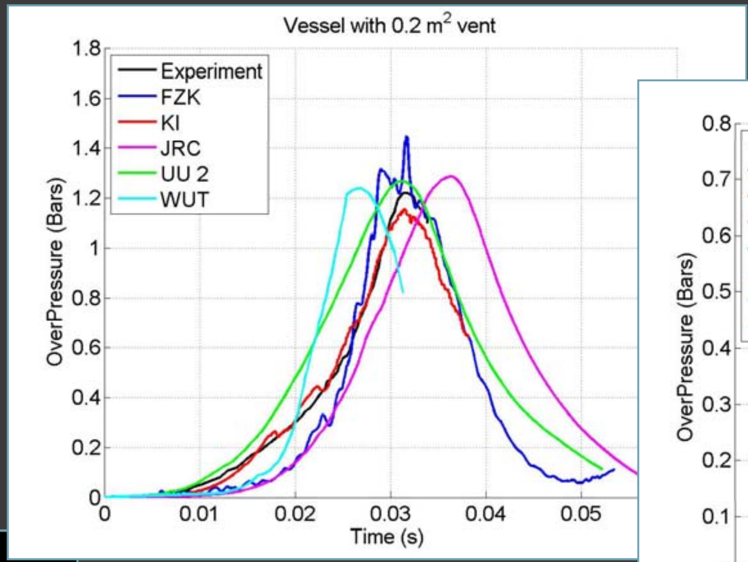


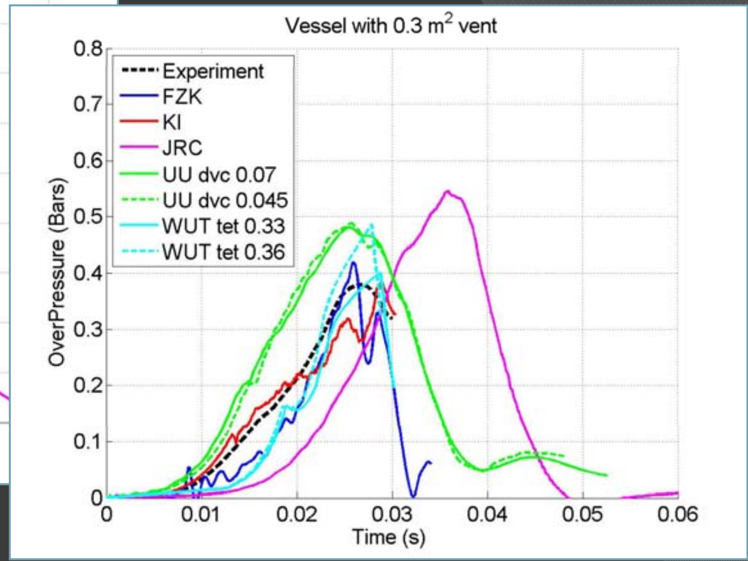
Address: Mitigation by venting, deflagration in outflow during venting, pressure development

5 partners
Turbulence: Empirical correlations – RANS - LES
Combustion: Quasi-dimensional model with spherical flame – Adjusted speed – EDM – St(u´)

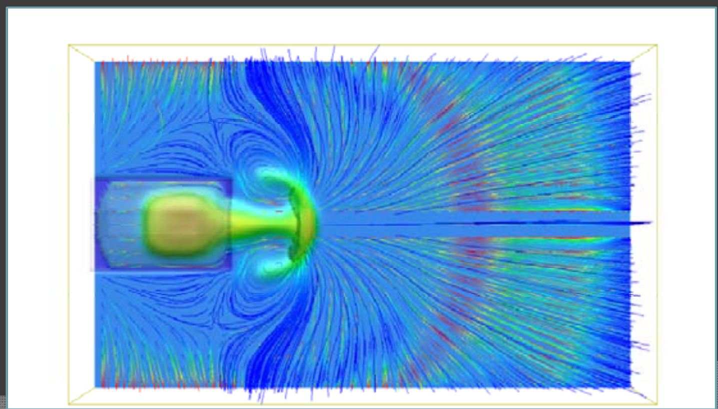
Pasman H.J., Groothuisen Th.M. and Gooijer P.H. in "*Loss Prevention and Safety Promotion in the Process Industries*", Ed. Buschman C.H., Elsevier, New-York, 1974, pp.185-189.

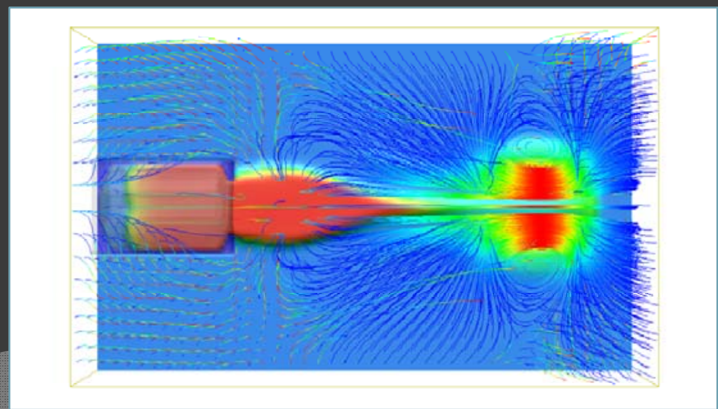






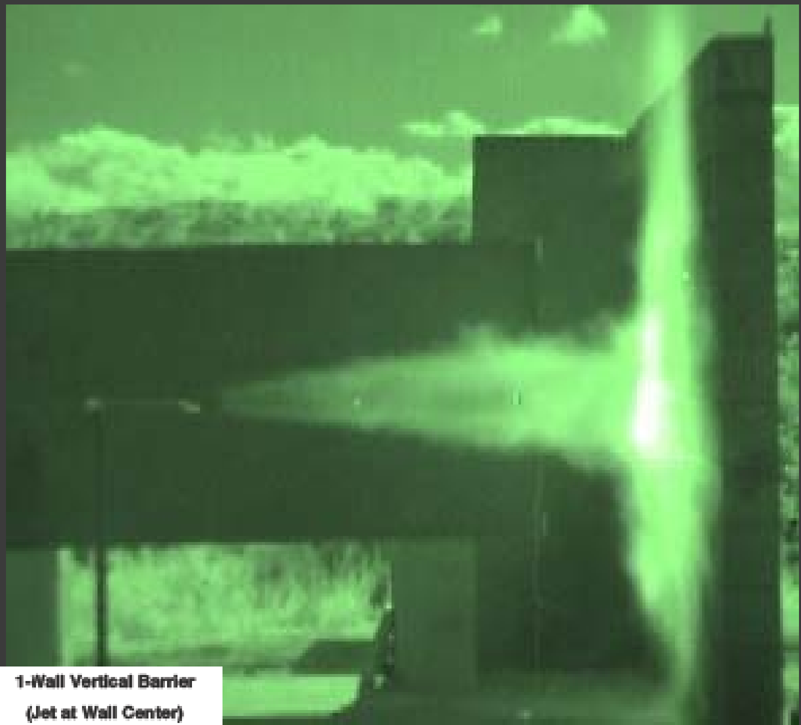
- Calculated pressure histories are in good agreement with experiments
- Requires special arrangement for rupture membrane
- Requires enlarged calculation domain due open boundaries

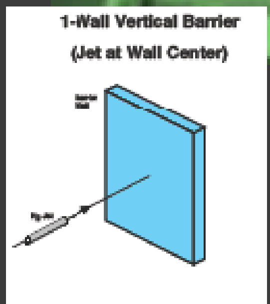




Barrier – wall interaction

SBEP V17





SNL test 1-07, nozzle 3.175 mm H_2 jet flame centred on a vertical wall from 13.79 MPa (2000 psi) cylinder

Case involved a single-barrier wall 2.44 x 2.44 m (8 x 8 ft) with jet flame impinging perpendicular to the wall and in the centre of the wall.

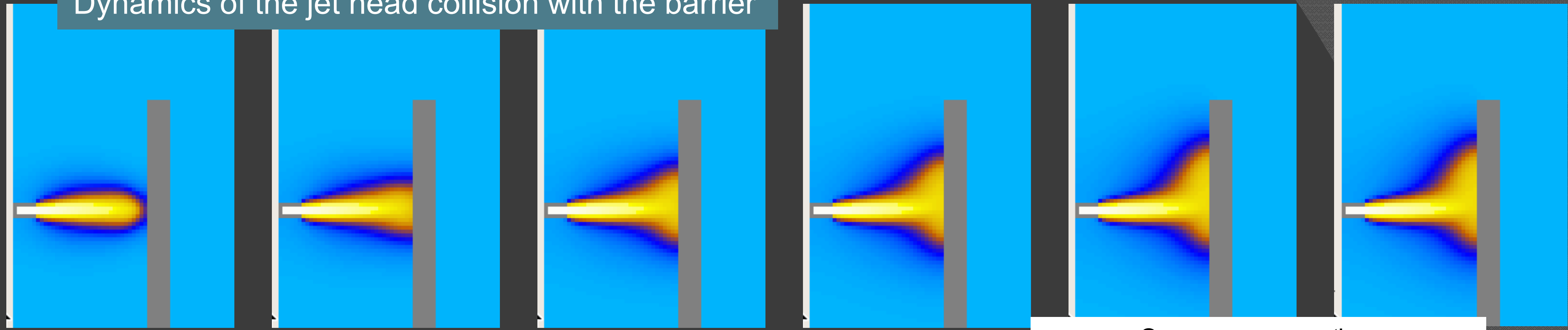
Address:

- Jet flames from high-pressure sources
- Explosion of H_2 during initial phase of jet impingement
- Barrier walls as potential mitigation mean for jet releases

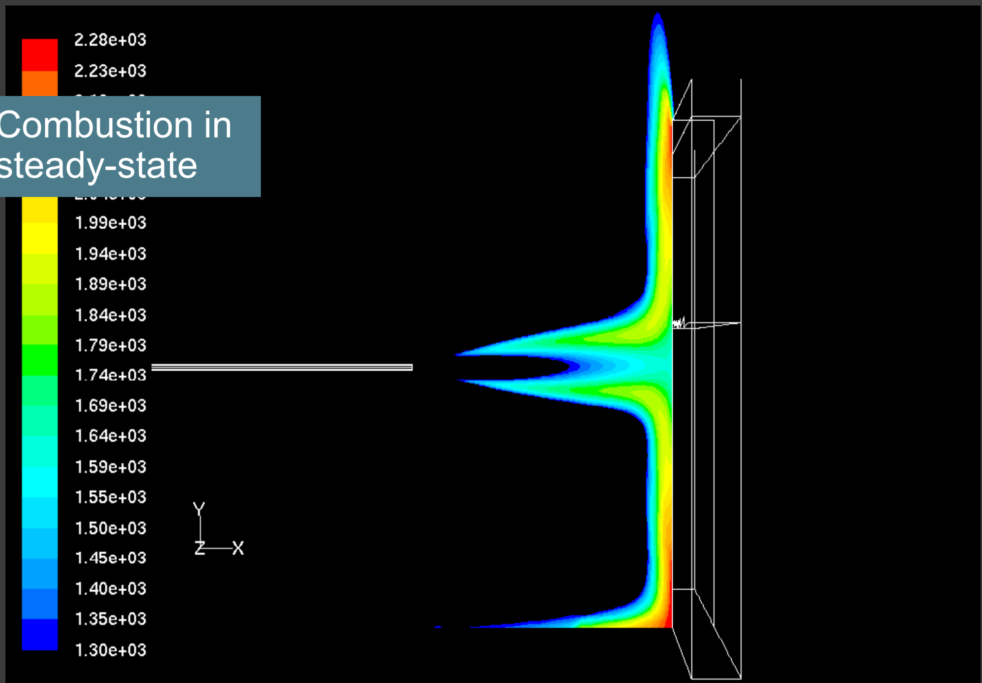
Resolution: Variable
Turbulence: RANS - LES
Combustion: Various(challenge, since combination of premixed and non-premixed regimes are realized)

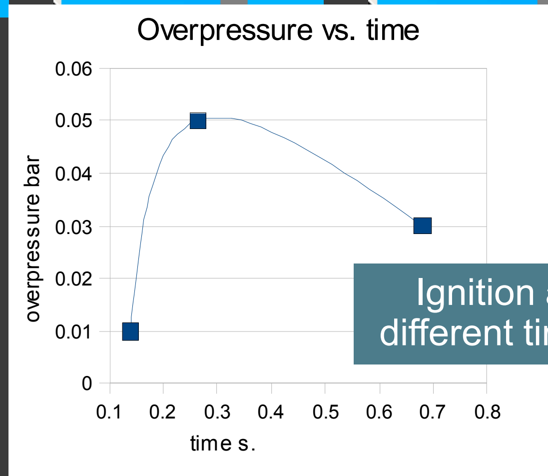
Houf, W. G., Evans, G. H., & Schefer, R. W. (2007). Analysis of jet flames and unignited jets from unintended releases of hydrogen. In 2nd ICHS, San Sebastian, Spain.

Dynamics of the jet head collision with the barrier



Combustion in steady-state





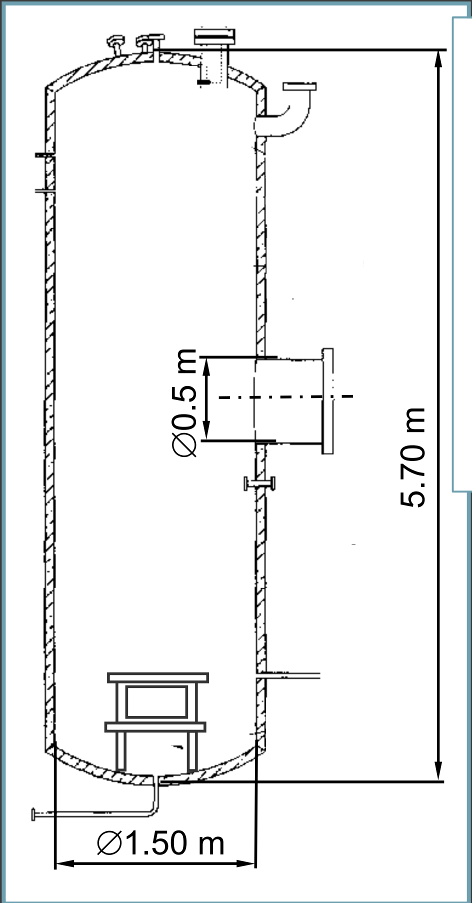
Ignition at different times

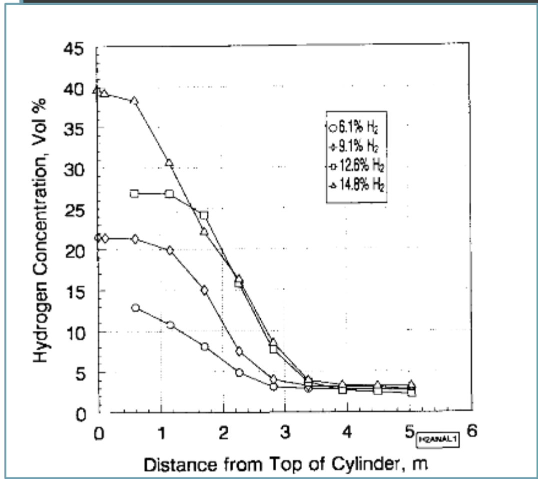
Comparison between simulations, experimental data and theoretical predictions shows that overall representation of the dispersion and combustion process has acceptable accuracy even on coarse grid, while takes very long time

For more accurate representation considerable efforts are required such as extensive grid refinements and usage of more advanced models, e.g. for equiv. nozzle replacement

Combustion of non-uniform mixtures

SBEP V18



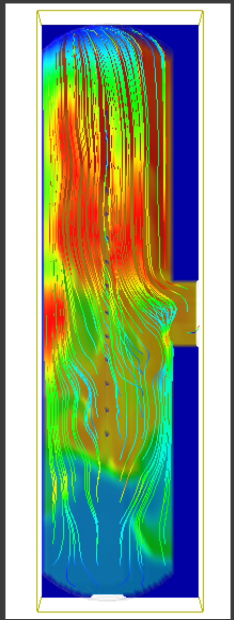


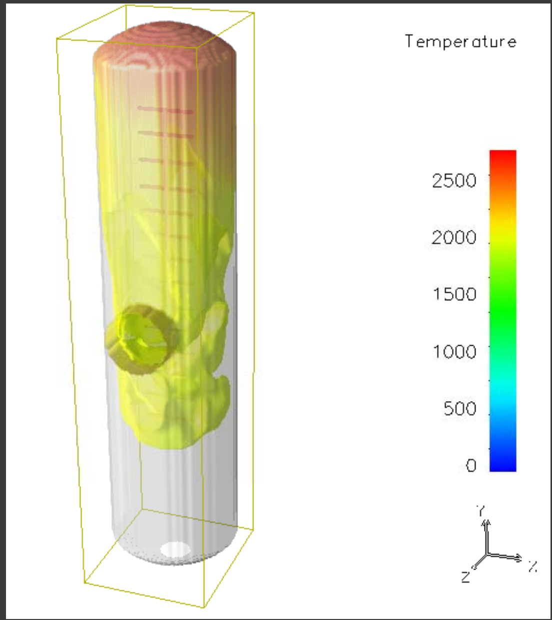
Cylindrical facility 10.7 m^3 (5.7-m high x 1.5 id)
Two combustion tests
uniform 12.8% H_2-air mixture
non-uniform (average 12.6%) with vertical stratification from 27% to 2.5%
Ignited at the top

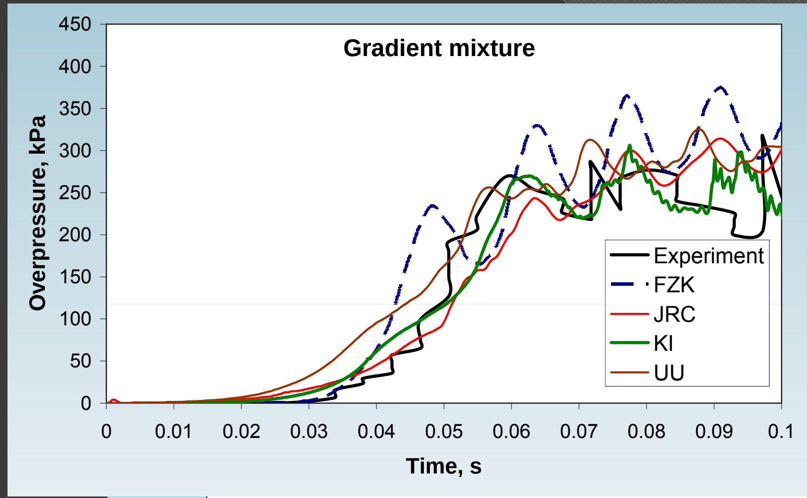
Address:
Influence of concentration gradient on combustion details
Combustion in closed volume
Combustion of lean mixtures

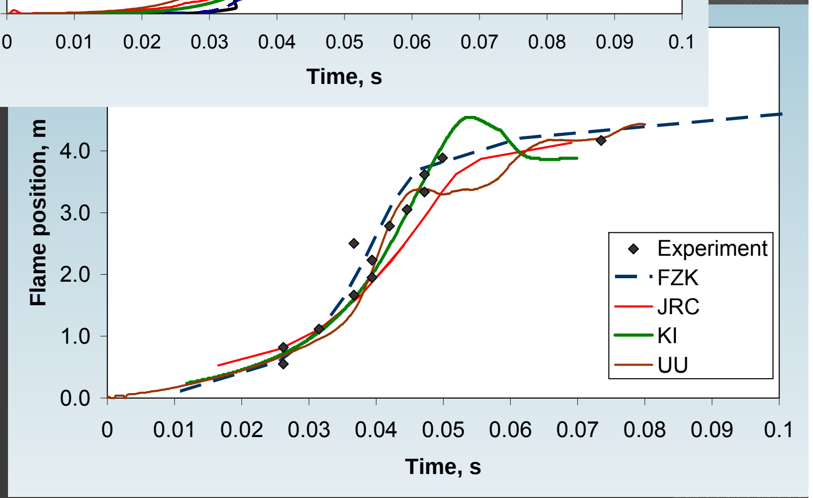
Resolution:
  Variable 2 cm – 20 cm
Turbulence:
  Algebraic – RANS - LES
Combustion:
  Adjusted speed – EBU – St(u´)

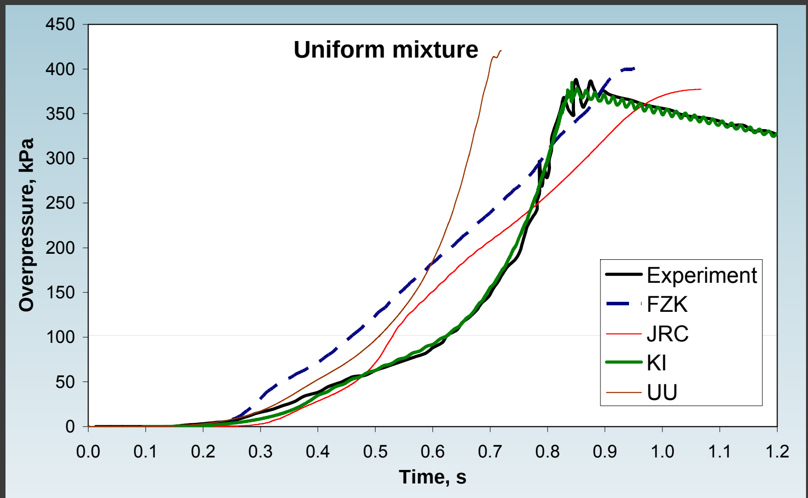
Whitehouse D.R., Greig D.R., Koroll G.W., Combustion of stratified hydrogen-air mixtures in the 10.7 m3 Combustion Test Facility cylinder. *Nuclear Engineering and Design*, V.166, Iss.3, Nov., pp.453-62, 1996.











Satisfactorily simulate hydrogen deflagration dynamics in realistic non-uniform hydrogen-air mixtures

Require models’ improvement for lean hydrogen-air deflagrations (flame speed in uniform case ≈ 8 m/s, in non-uniform ≈ 80 m/s), i.e., models for transient laminar-to-turbulent regime

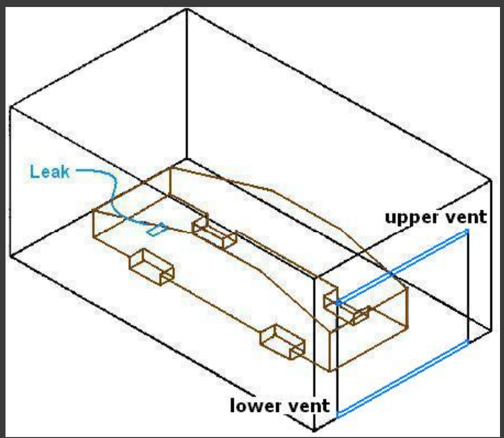
Application oriented simulations

Garage environment

SBEP V20 and V21

Facility GARAGE at CEA:
- Turbulent buoyant jet
- Volume flow rate 712.2 l/min
- Mass flow rate 1.99 g/s
- Injection diameter 0.02 m
- Release (upward) duration 121 s
- Injection velocity 37.78 m/s

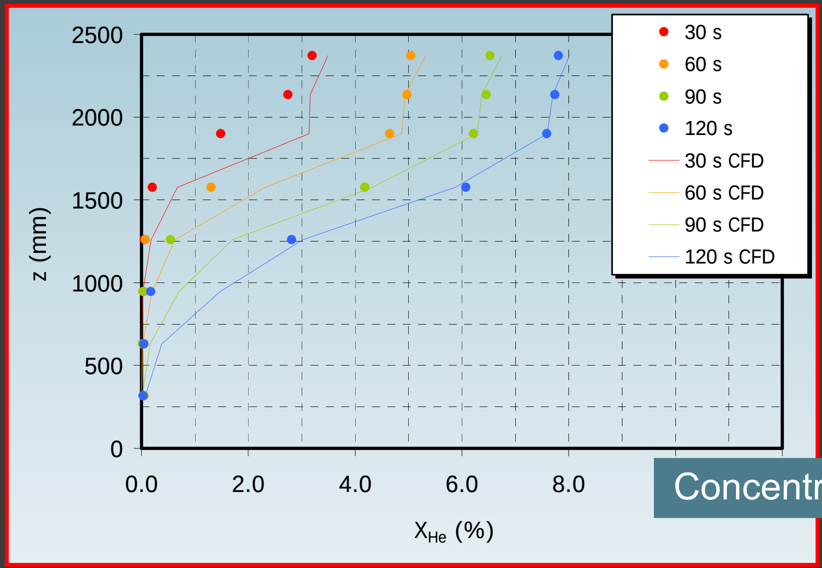
Determine the most appropriate turbulence model for the simulation of H_2 release and dispersion foe vehicles stored in residential garages
Compare different grid methodologies/approaches and boundary conditions applied

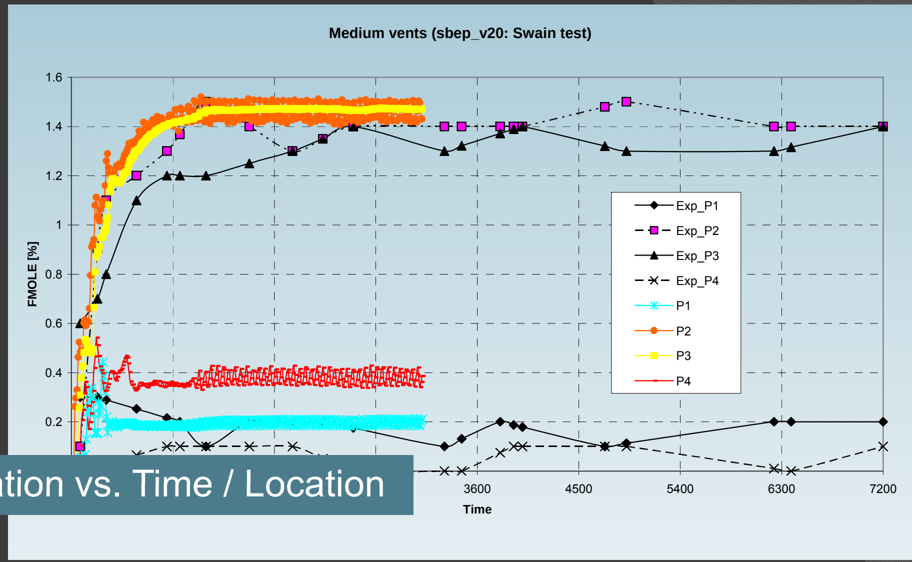


SBEP proposal and specification, NCSRD:
- 7.200 Lt/hr Helium for 2 hours
- Case 1: 2.5 inches (6.35 cm) top and bottom door vents
- Case 2: 9.5 inches (24.13 cm) top and bottom door vents
- Case 3: 19.5 inches (49.53 cm) top and bottom door vents

- He release area: under the car, 0.1 x 0.2 m
- He inflow velocity: 0.1 m/s
- He mass flow rate: $3.27 \cdot 10^{-4}$ kg/s

Swain M.R. "Addendum to Hydrogen Vehicle Safety Report: Residential Garage Safety Assessment", University of Miami, 1998

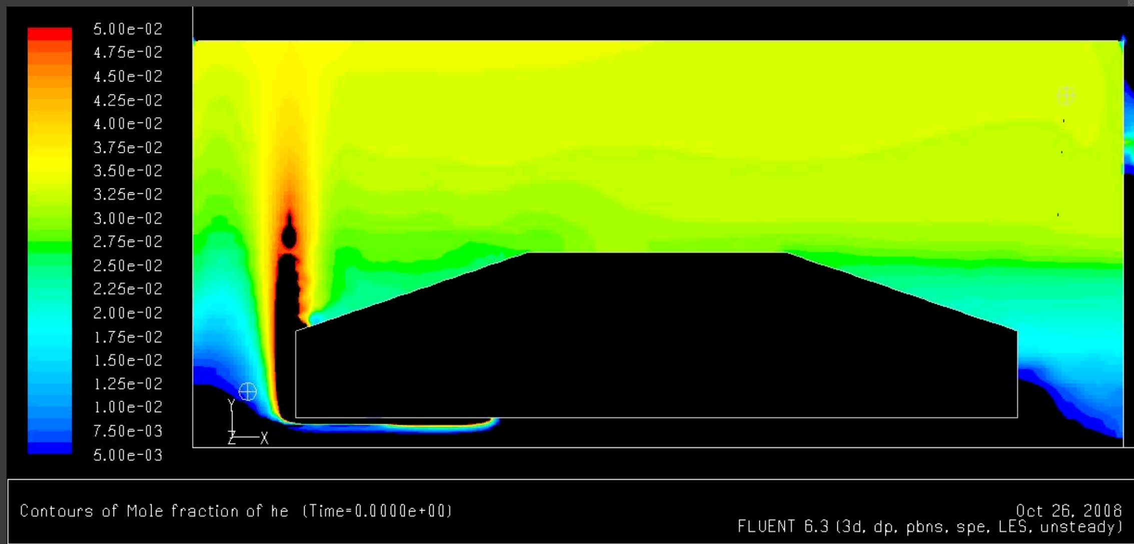




Concentration vs. Time / Location

Generally high quality of the numerical prediction of H_2 concentration development in both RANS and LES simulations

Adequate accounting of ventilation openings



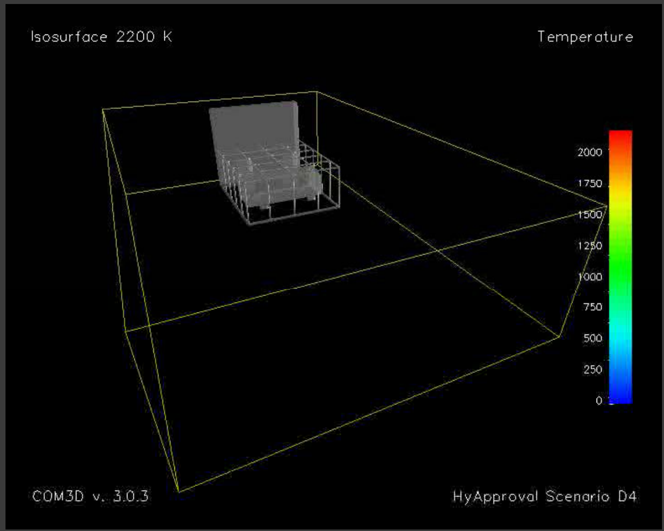
H_2 release ignited in a simulated vehicle refueling environment

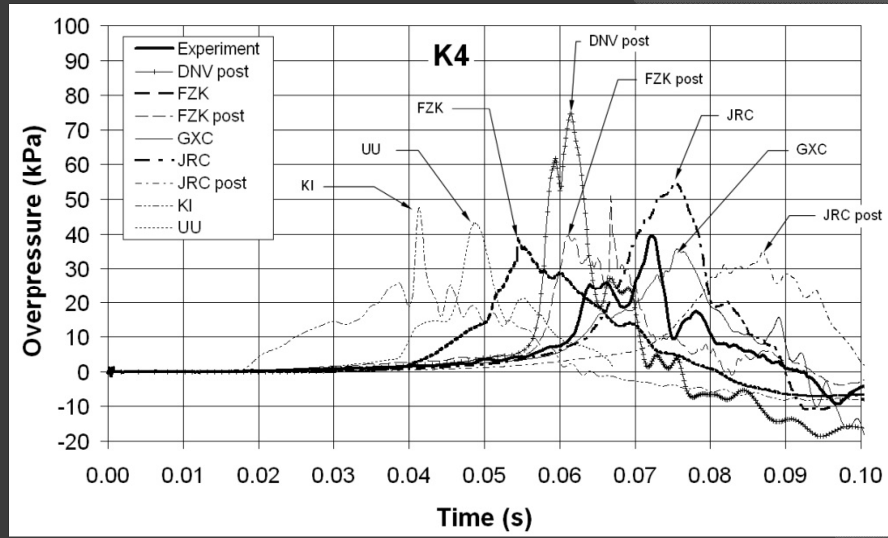
SBEP V07

7 partners
Blind simulation was performed
Resolution: locally 3 cm – 1 m
Turbulence: Algebraic - RANS – LES
Combustion: Adjusted speed – EDM – St(u´)

Shirvill, L.C., Royle, M. and Roberts, T.A. HYDROGEN RELEASES IGNITED IN A SIMULATED VEHICLE REFUELLING ENVIRONMENT , Int. Conf. on Hydrogen Safety 2, San Sebastian, Sept. 2007

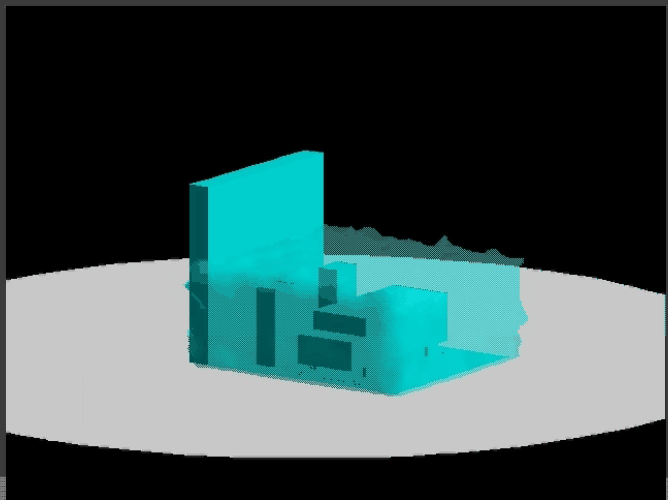
Realistic conditions (scale, environment, H_2 inventory). Generic H_2 refueling station. Development of worst-case scenario (premixed case)

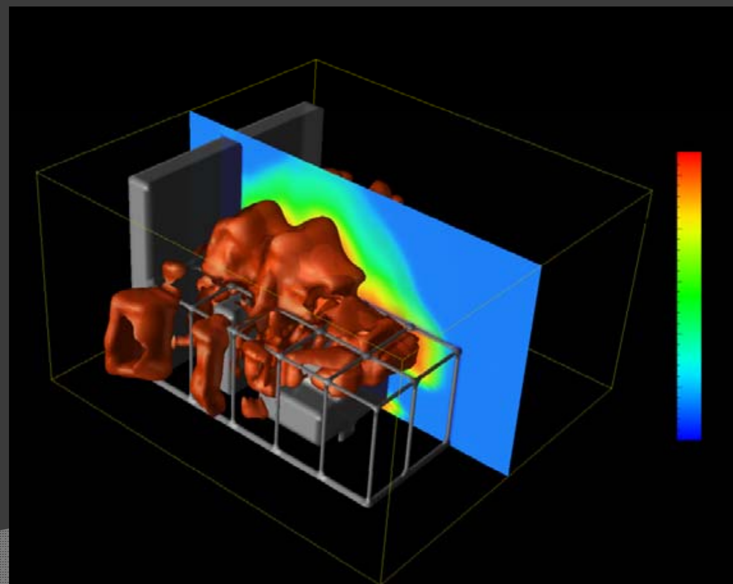




Reasonable agreement in pressure load

Considerable scatter in time-of-arrival for pressure wave, due to differences in combustion and ignition models





Combustion in model of road tunnel

SBEP V12

1/5 real-scale experiments on hydrogen-air deflagration in tunnel
30% H_2-air mixture in 37 m^3 with model of 4 cars

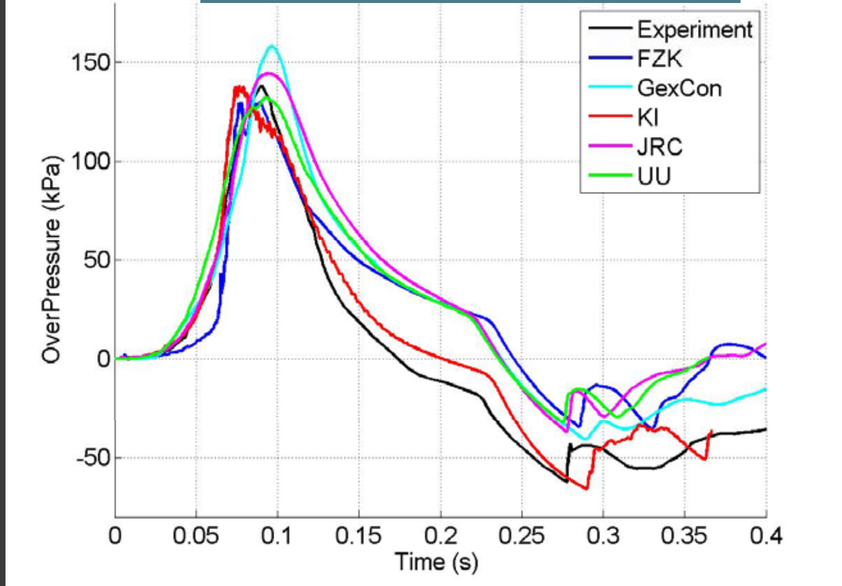
Deflagration process development with pressure dynamics with and without vehicle models for 30 % H_2-air homogeneous mixture

5 codes:
Resolution: 5 cm – 1 m (cells 150 000 – 2 500 000)
Turbulence: Algebraic - RANS – LES
Combustion: Adjusted speed – EDM – St(u´)

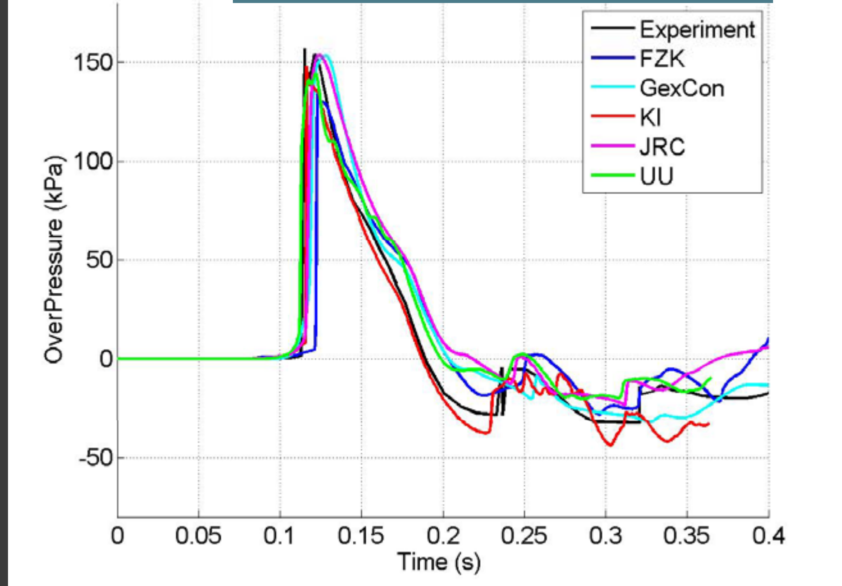
Groethe, M., Merilo, E., Colton, J., Chiba, S., Sato, Y., and Iwabuchi, H., ICHS, Pisa, Italy, 8-10 September 2005. ISBN 88-8492-314-X

Overpressures for case with obstacles 30% H_2

Transducer at 1.0 m



Transducer at 30.4 m

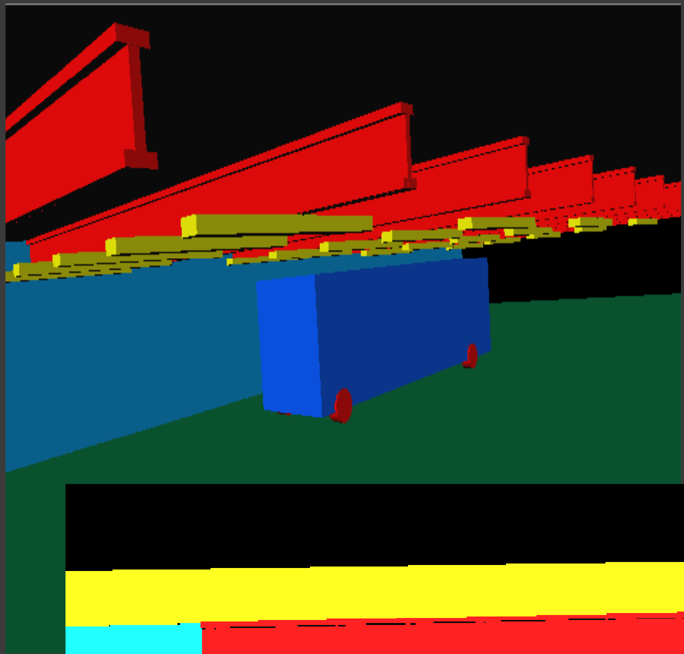


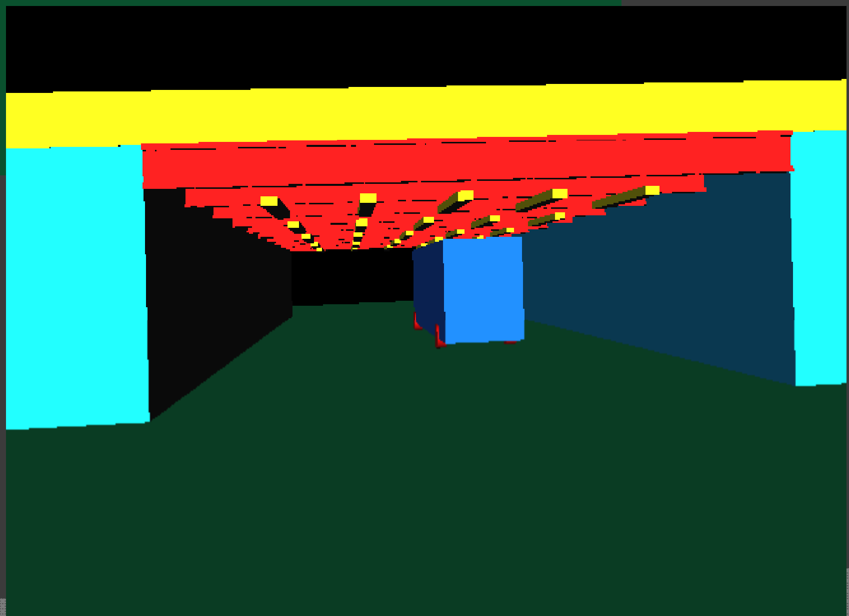
- Correct value of the pressure peaks
- Correct time of arrival of the blast wave
- Correct speed of propagation of the blast wave
- Precision of the pressure peaks is good

CFD tools are capable to describe combustion in a tunnel environment

Problems: rate of the pressure rise and the maximum pressures
Possible causes: mesh resolution, the numerical scheme and flame acceleration model

Direct connections from CFD to (Q)RA





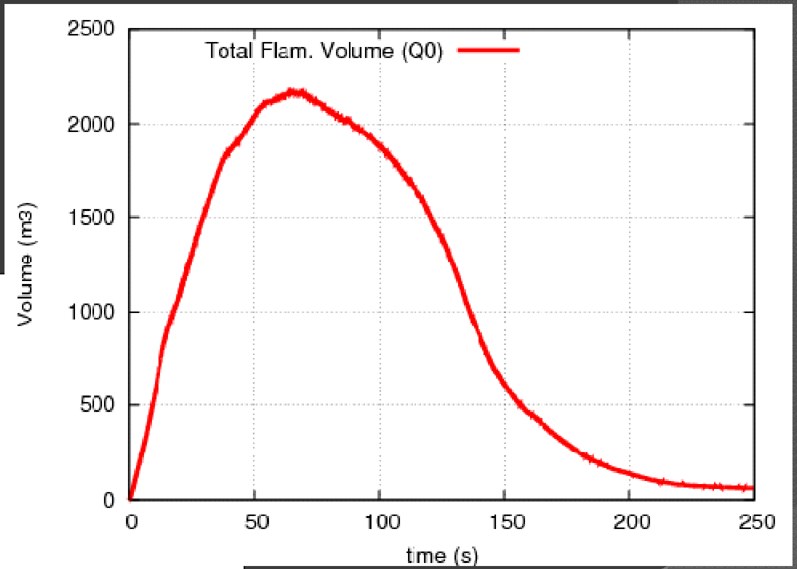
In the frames of internal project HyTunnel;
SBEP V11 and V15

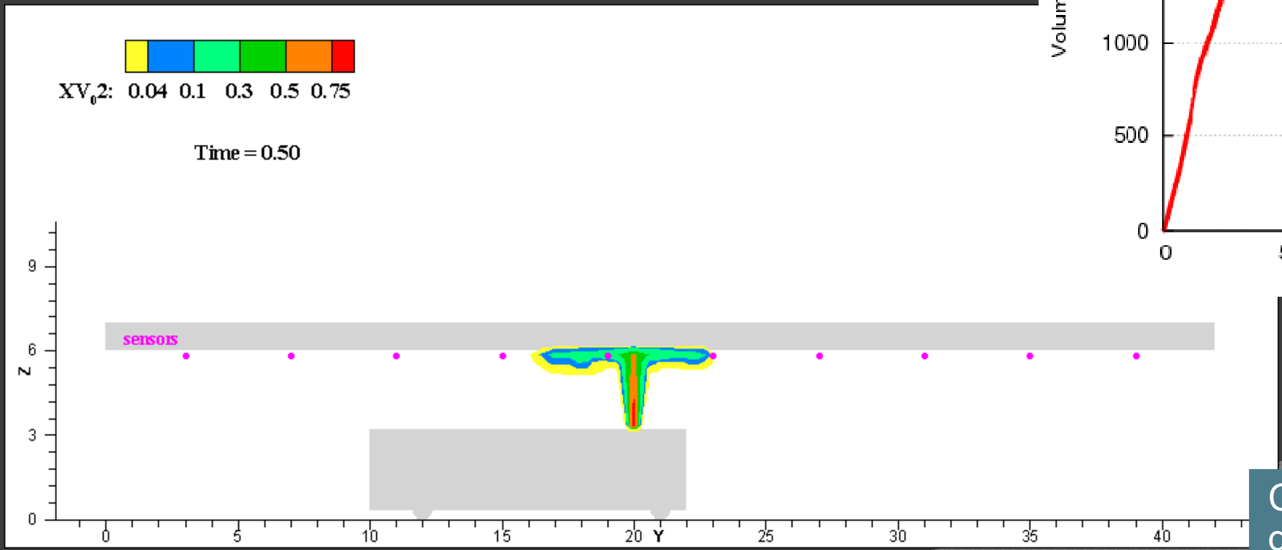
Systematic study of tunnel accident scenario development
- H_2 inventory
- release location
- ignition location
- ignition time
- influence of environment details (obstruction, confinement)

Geometry environment an underpass below a highway:
- 0.8 m H-beams every 4m (10 cm thick with 30 cm ends)
- Length = 40 m, Width = 15 m, Heigth = 5 m
- Bus at pos (8 m, 10 m, 0 m) with size (3 m, 12 m, 3.5 m)
- Light armature: 4 x 0.4 x 0.2 m located as shown

	Simulation	Type
1	20 kg released from a tank with 350 bar pressure (position 9m, 20m, 3.3m)	Base Case
2	Jet hits light armature (position 10m, 20m, 3.3m)	Sensitivity 1
3	Original release location (flat ceiling at z=5m, shift of sensors to 4.8m height)	Sensitivity 2
4	5 kg H2 released (1 tank), original geometry and release position	Sensitivity 3

- Data on dynamic of flammable cloud
- Data on pressure loads for different scenario realizations





Cartesian non-equidistant grid ~ 200.000 cells

What are the lessons we have learned

Database for hydrogen safety with experimental data and partially supplemented by simulations was created and is available

The considered cases were simulated within the following computational limitations
- grids with spatial resolution from 1 cm – 10 cm
- for such resolutions grid size was in the range 50 000 – 1 000 000 cells
- calculation time ranged from several hours to 1-2 days
- computers used were from ordinary PC to PC clusters up to 50 CPUs

Thus it was demonstrated that many practically important cases can be successfully simulated with level of authenticity necessary for safety analysis

While …

All calculations were made for known results (excluding one), thus value of these simulations is in some way reduced, blind case induced larger scattering in the predictions

All of the cases where specially designed set-ups without details existing in real life (e.g., small-scale obstructions), which can affect dispersion and combustion processes

What we have learned from those lessons

Non-reactive systems:

• Generally good quality of simulations
• In turbulent cases often LES and RANS give similar quality, in cases when LES is required it demands better resolution
• Applicability of LES in each particular case requires additional approvement
• Problems by modeling of high momentum jets (commonly used approach to replace nozzle area by equivalent source requires further development)
• Modeling of liquid spills require further development

Reactive systems:

• For premixed cases approach which uses St(u´) seems to be most effective and provides generally good quality, including non-uniform mixtures and vented deflagrations
• Generally both RANS and LES approaches provide reliable data on the turbulence necessary for the St(u´) model
• Initial phase of flame acceleration, including transient from laminar to turbulent burning is still not well established
• For non-premixed cases the simple models such, e.g. EDM produce reasonable results, since for the practical cases regime of diffusion flame gives adequate approximation
• Combination of premixed + non-premixed cases requires further development and validation of the specialized models
• Simulation of steady state detonation with the appropriate models produces good results
• DDT requires considerably more sophisticated models and better resolution