Karlsruher Institut für Technologie

Numerical analytical code development at Karlsruhe Institute of Technology KIT

Thomas Jordan, IKET, H2 Group

Technical session 1 – Analytical and experimental research
Fukushima Research Conference – Workshop on Nuclear Hydrogen Safety FRCHS2019
17-18 October, 2019

Institute for Nuclear and Energy Technology

Outline

- **INTRODUCTION**
- **GASFLOW-MPI**
  - Overview
  - Geometry modelling and mesh generation
  - Combustion modelling
  - Film modelling
- **COM3D**
  - Overview
  - Adaptive Mesh Refinement
  - Fluid-Structure Interaction
- **CLOSURE**

INTRODUCTION

History of Nuclear Research in Karlsruhe

1956: Reactor Construction and Operating Company mbH
Nuclear Research Center Karlsruhe
1995: Research Center Karlsruhe
2009: Karlsruhe Institute for Technology after merger with University

- 1961: Research reactor FR2 44 MW_{th}, operation until 1981
- 1965: Multipurpose research reactor MZFR, 58 MW_{e}, operation until 1984
- 1971: Compact sodium-cooled nuclear reactor plant Karlsruhe (KNK) 21 MW_{e}, operation KNK2 until 1991
- 1971: Reprocessing plant WAK for 35 t/a, operation until 1990

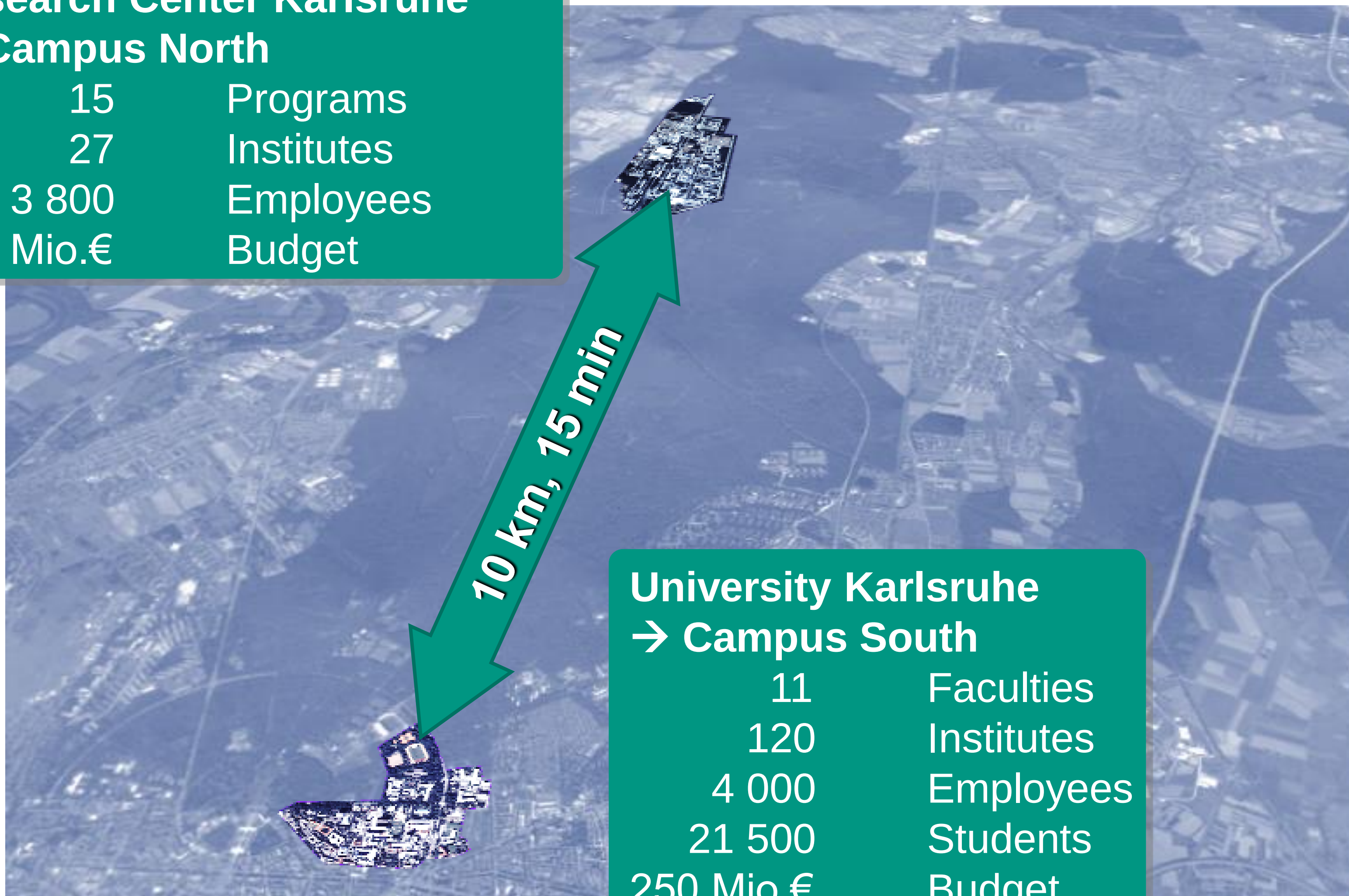
Japanese experts visit the Hydrogen Test Center HYKA

Merger of the University Karlsruhe with the Research Center Karlsruhe in 2009 →

KIT Karlsruhe Institute of Technology

Research Center Karlsruhe
→ Campus North

15	Programs
27	Institutes
3 800	Employees
305 Mio.€	Budget



University Karlsruhe
→ Campus South

11	Faculties
120	Institutes
4 000	Employees
21 500	Students
250 Mio.€	Budget

Institute for Nuclear and Energy Technology (IKET) Hydrogen Group

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Methods and Tools for Hydrogen Safety
Safety of Flammable Gases, Dusts and Hybrid Mixtures

Theory – Analytical Tools

GASFLOW-MPI
COM3D

design → **Experiments**

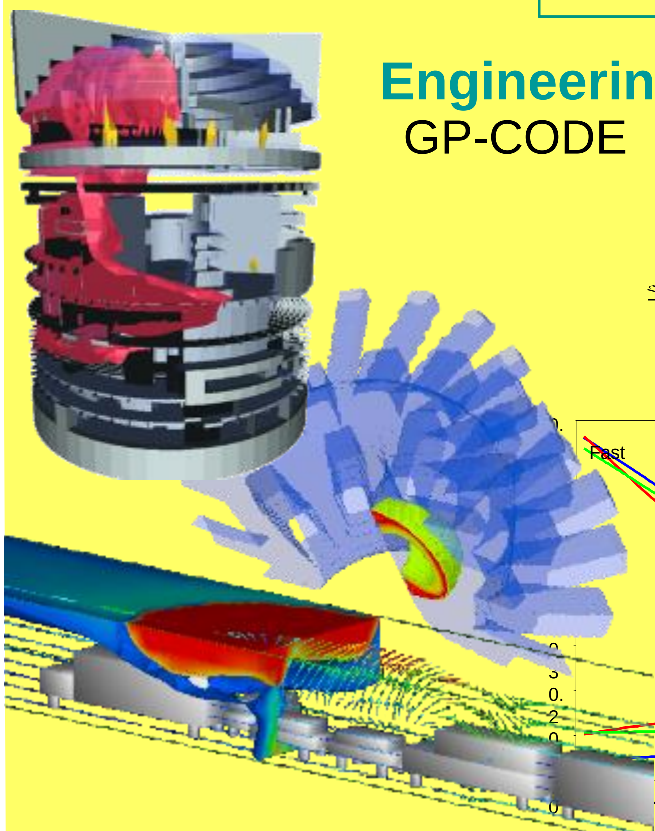
← *validate*

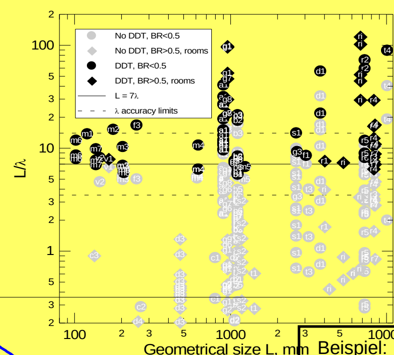
Hydrogen
Test Center

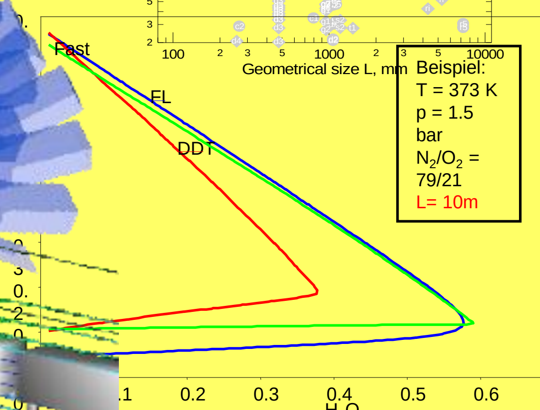
implement

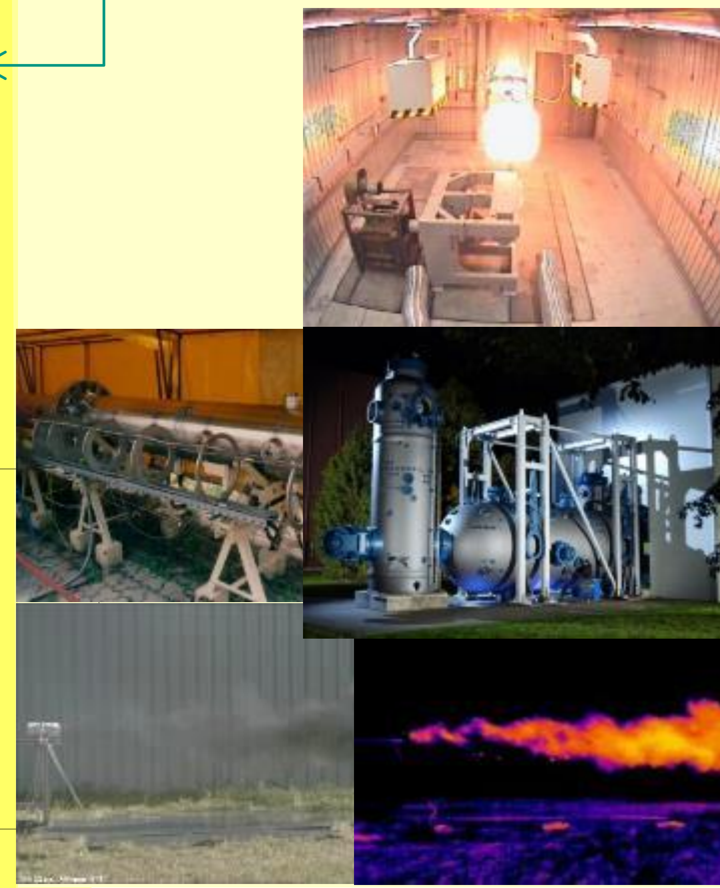
Models – Engineering Correlations

GP-CODE







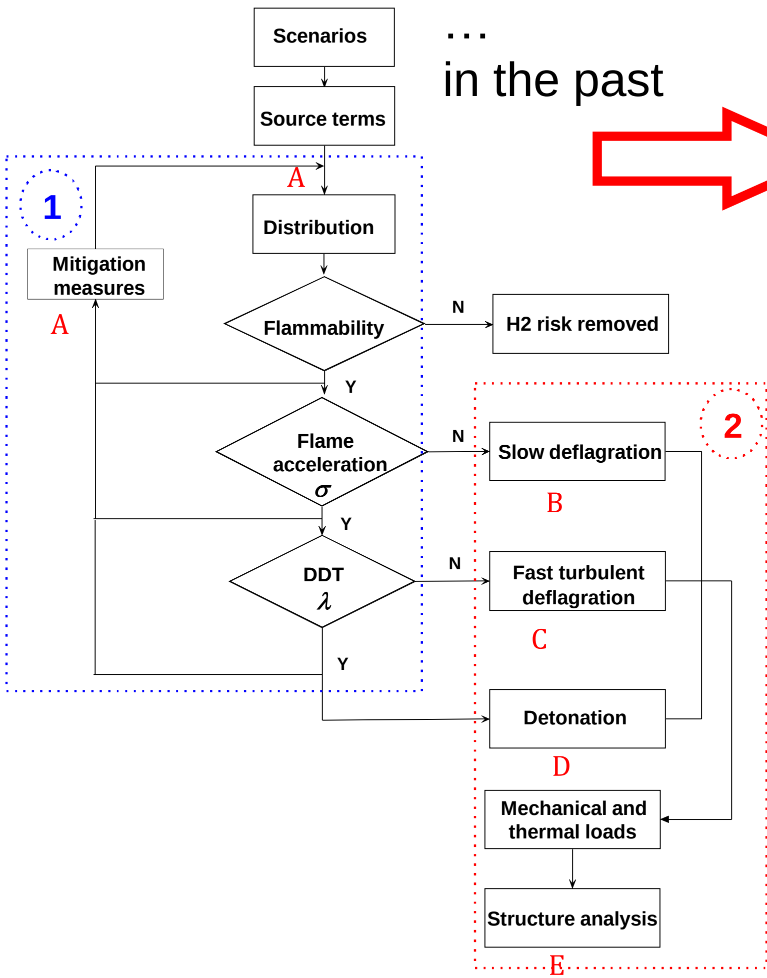


State-of-the-Art Containment Safety Code

GASFLOW-MPI

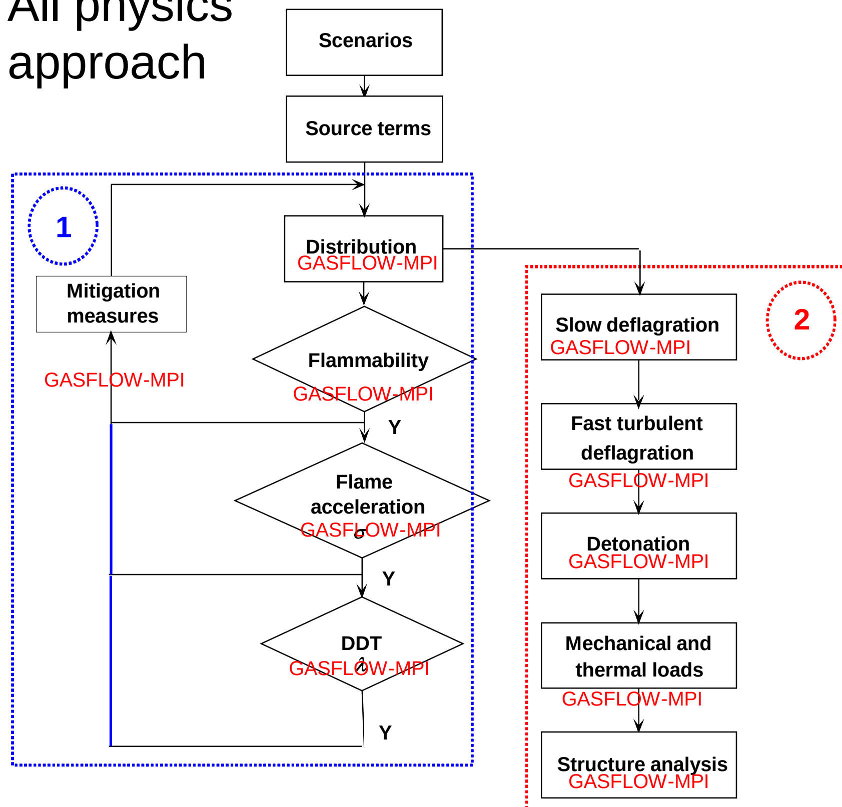
GASFLOW-MPI: “One-Stop-Shopping”
All-speed CFD code for Hydrogen Safety Analysis

Simulate flows at broad Mach number regimes with one all-speed numerical solver



… in the past

All-speed, All physics approach



GASFLOW-MPI: Features I/III

- **Flexible geometrical modeling capability**
  - Obstacles
  - Walls and rupture discs
  - Holes
  - Fractional Area/Volume Object Representation (FAVOR)
  - Geometric modeler
- **Flexible structured mesh capability**
  - Cartesian
  - Cylindrical
  - Non-uniform mesh
  - Multi-block
  - Immersed boundary
- **Flexible boundary conditions**
  - Global BC
  - PBC, VBC, MBC, CBC
  - Periodic boundary condition
  - Absorbing boundary condition
- **Proven technology of solving N-S equations and accurate numerics**
  - ICE'd ALE
  - 1st order upwind
  - 2nd order Van Leer
  - Higher order schemes
- **Cutting-edge, scalable and powerful high performance computing capabilities**
  - PETSc
  - Third-party pre-conditioners and solvers

available | Under development | plan

GASFLOW-MPI: Features II/III

- **Turbulence modelling**
  - Algebraic
  - κ-ε
  - κ-ω and SST κ-ω
  - DES
  - LES
- **Heat and mass transfer, radiation model**
  - Conjugate heat transfer
  - 1-D heat conduction (slab, wall, sink)
  - Radiation model
  - 3-D heat conduction (slab, wall, sink)
- **Multiphase flow**
  - Homogeneous equilibrium model
  - Lagrangian Discrete multiphase model
  - Eulerian multiphase model
- **Combustion models**
  - Eddy break-up
  - Eddy dissipation
  - Arrhenius for detonation
  - Various correlations for turbulent flame velocity
- **Material properties**
  - 25 Gas species
  - 20 solid materials
  - Porous media

available | Under development | plan

GASFLOW-MPI: Features III/III

- Unique features for large scale industrial applications

Simplified pipe model	Ignitor model	Recombiner model	Sump model	Fan model	Pre-expansion model
Static film model	Spray model based on HEM	Xenon decay model	Sigma and DDT criteria for H2 explosion risk analysis		
Aerosol model	Lagragian dust transportation	Spray model based on Eulerian Multiphase model			
Dynamic film model	Dust modeling based on Discrete Multiphase model	Spray model based on Discrete Multiphase model			

- Pre-processor, Post-processor and data export

pyscan	netcdf4	Data format to Third-party post-processing tools	Automatic mesh generation via CAD import

available | Under development | plan

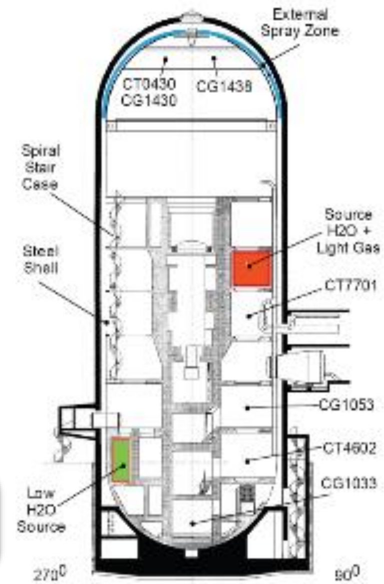
GASFLOW-MPI: Some Validation References

Karlsruhe Institute of Technology

GASFLOW validation library

HYKA (Germany)

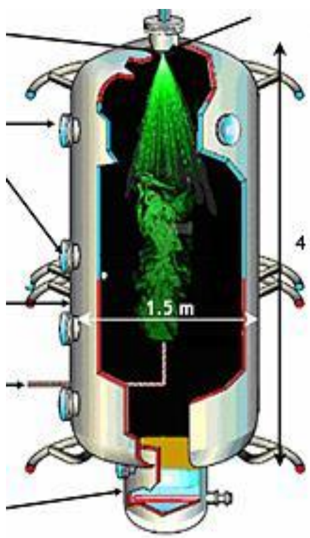
PANDA (Switzerland)



Cut through HDR containment with setup for HDR test E11.2

HDR (Germany)

MISTRA (France)



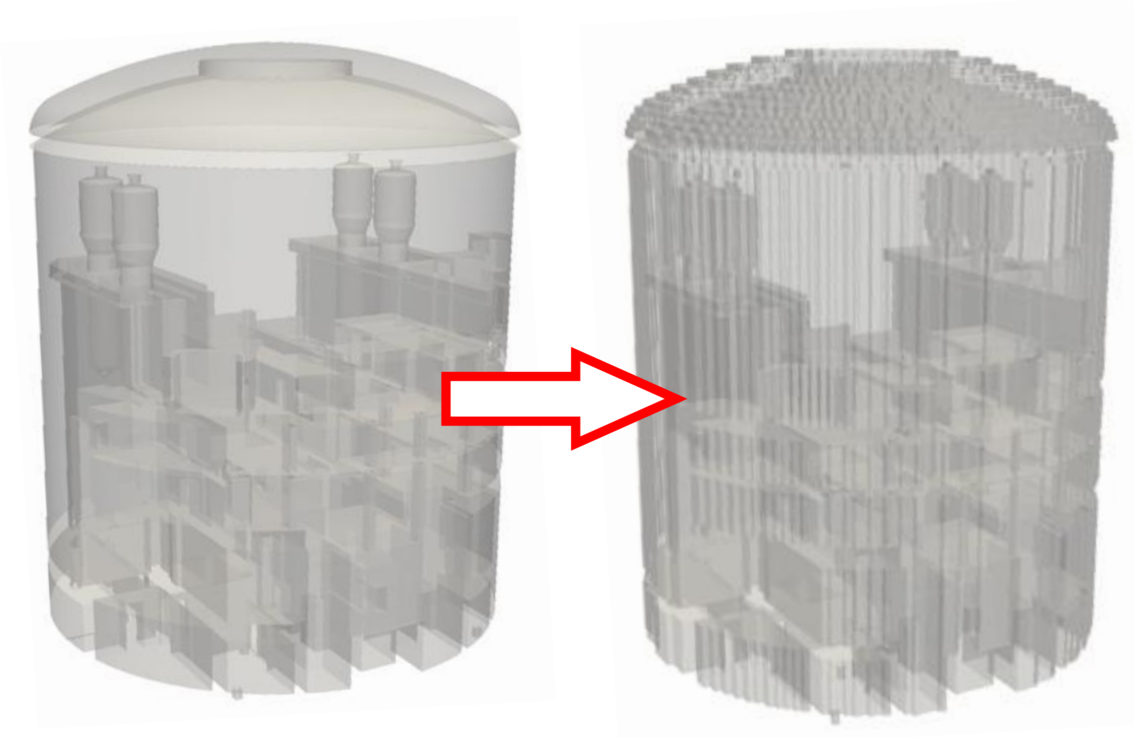
TOSQAN (France)

THAI (Germany)

SARNET

GASFLOW-MPI: Automatic Mesh Generation Containment Geometry Modelling

- Large volumes (~100.000 m^3)
- Complex multi-connected inside structure
- Mitigation measures



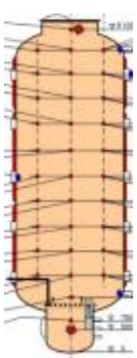
- ✓ Use of any standard CAD format IGES, STEP, STL,…
- ✓ Selection of spatial resolution
- ✓ Automatic wall, obstacle generation and material association, and optimized discretization

Example APR1400:

- 37 individual rooms, including RPV, steam generators and pumps
- total free volume of ~ 48.000 m^3
- Passive Autocatalytic Recombiner equipment
- Ignitor system
- Containment spray system

GASFLOW-MPI: Validation of combustion models

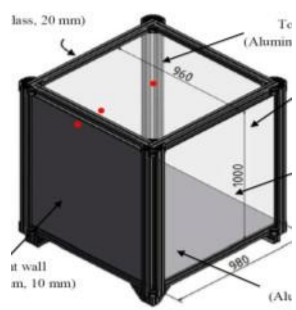
Validation	Facility	Year	Publications
Slow deflagration	THAI HYKA A2	**2017** **2017**	**J. Xiao, M. Kuznetsov.** *NURETH-17*, September 3 – 8, 2017 **J. Xiao, M. Kuznetsov.**
Fast deflagration	HYKA jet fire ENACCEF	**2016** **2015**	**J. Xiao, M. Kuznetsov.** *8th International Seminar on Fire and Explosion Hazards*, Hefei, China, April 25-28, 2016 **J. Xiao, M. Kuznetsov.** *International Journal of Hydrogen Energy* 09/2015; 40(38):13106–13120.
Detonation	KIT Detonation tube RUT Hemi-spherical balloon	**2016** **2016** **2016**	**J. Xiao, M. Kuznetsov.** *International Journal of Hydrogen Energy* March 2017, 42(12): 8346–8368. **J. Xiao, M. Kuznetsov.** *International Journal of Hydrogen Energy* March 2017, 42(12): 8369–8381. **J. Xiao, M. Kuznetsov.** *ICONE 25*, July 2-6, 2017, Shanghai, China.
Flame acceleration DDT	KIT Detonation tube KIT Ring geometry	**2017** **2017**	**J. Xiao, M. Kuznetsov.** **J. Xiao, M. Kuznetsov.**



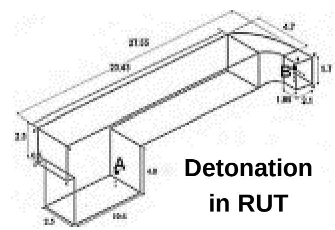
Slow deflagration in THAI

Slow deflagration HYKA A2

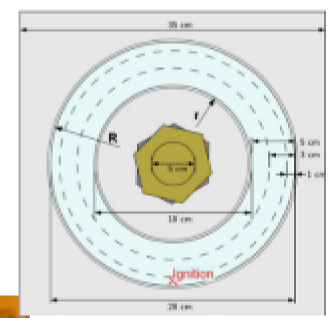
Fast deflagration in ENACCEF



KIT cubic for jet fire

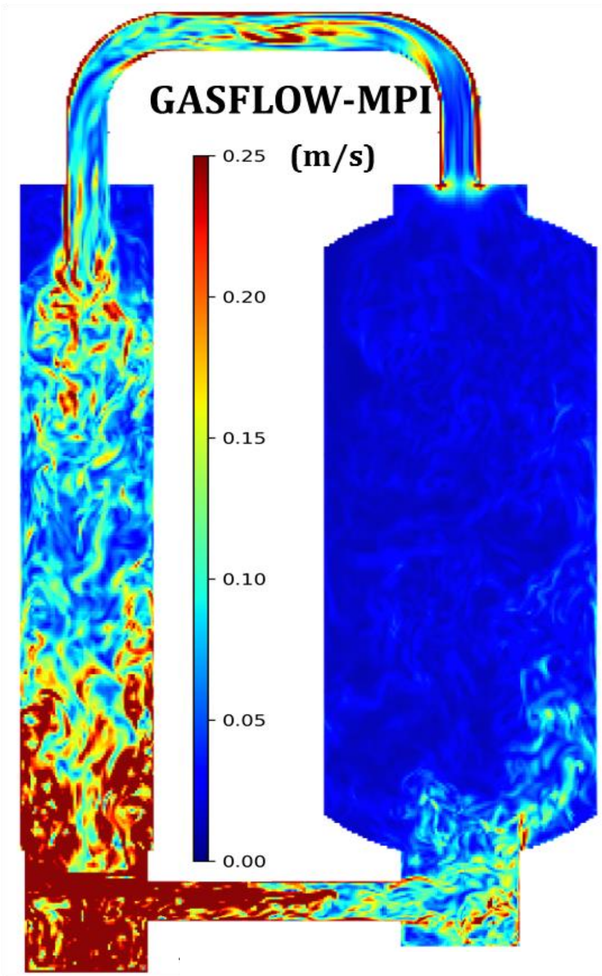


Detonation in RUT

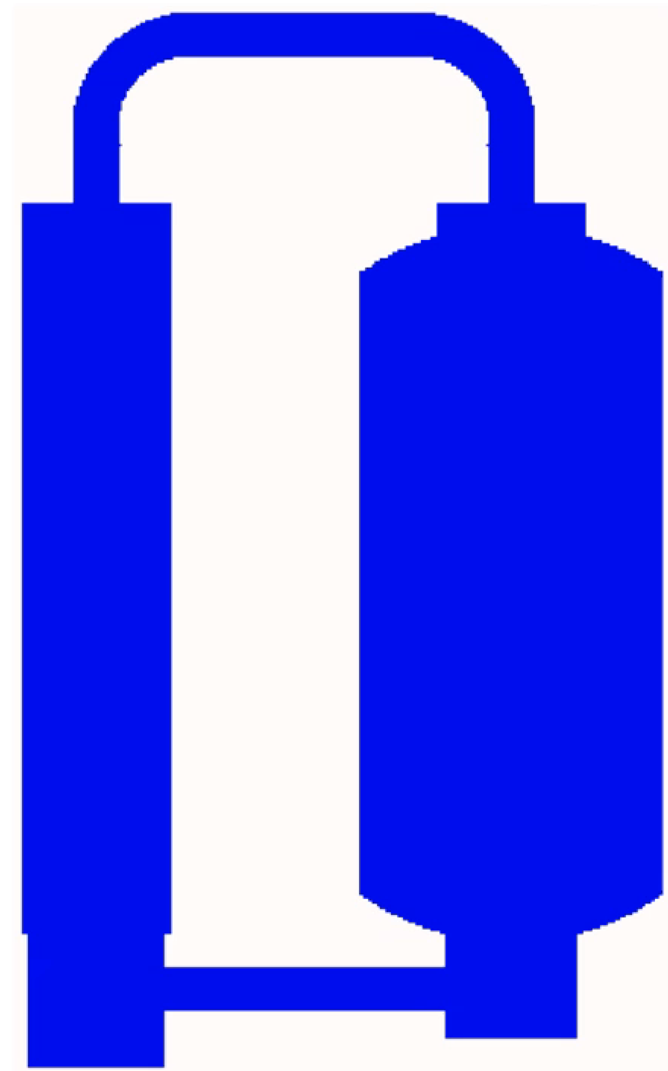


FA and DDT in ring-shaped geometry

GASFLOW-MPI: Slow deflagration with heat transfer in THAI-HD44

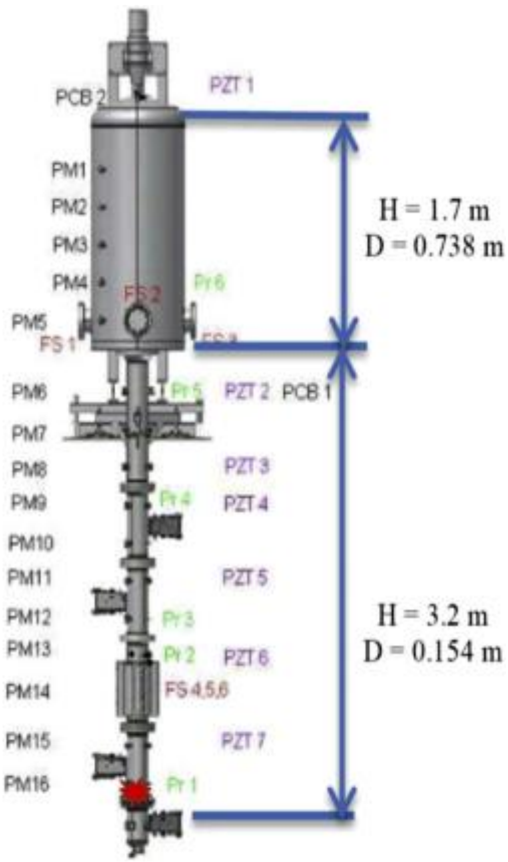


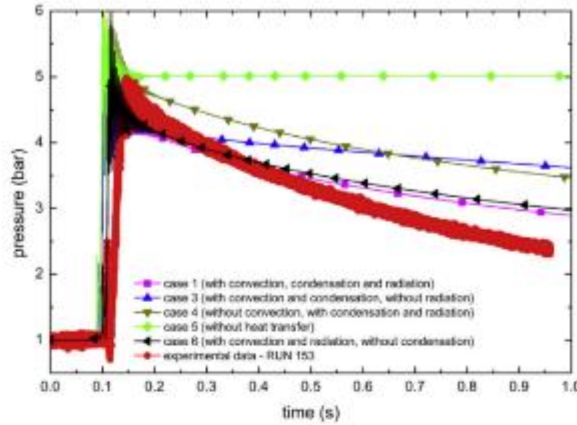
Turbulent velocity fluctuation (u') at 0 s before ignition

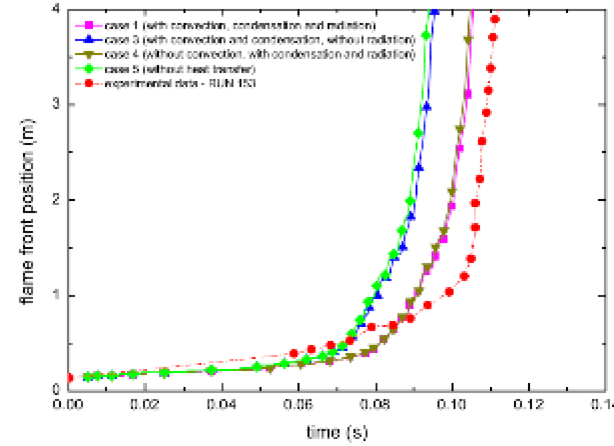


Flame propagation (0 s ~ 15 s)

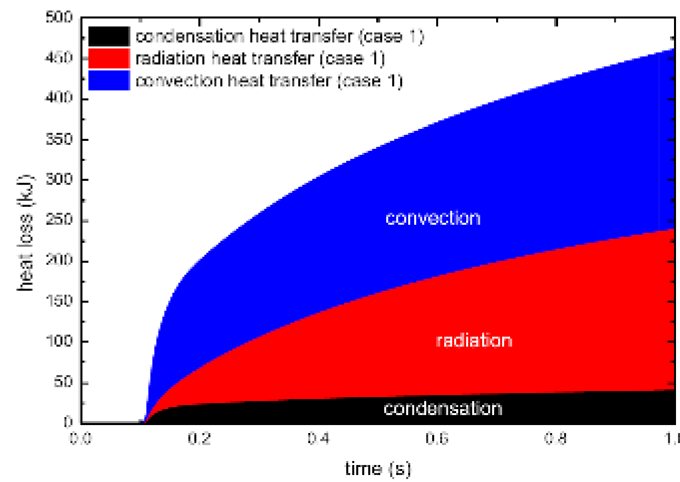
GASFLOW-MPI: Fast deflagration with heat transfer in ENACCEF





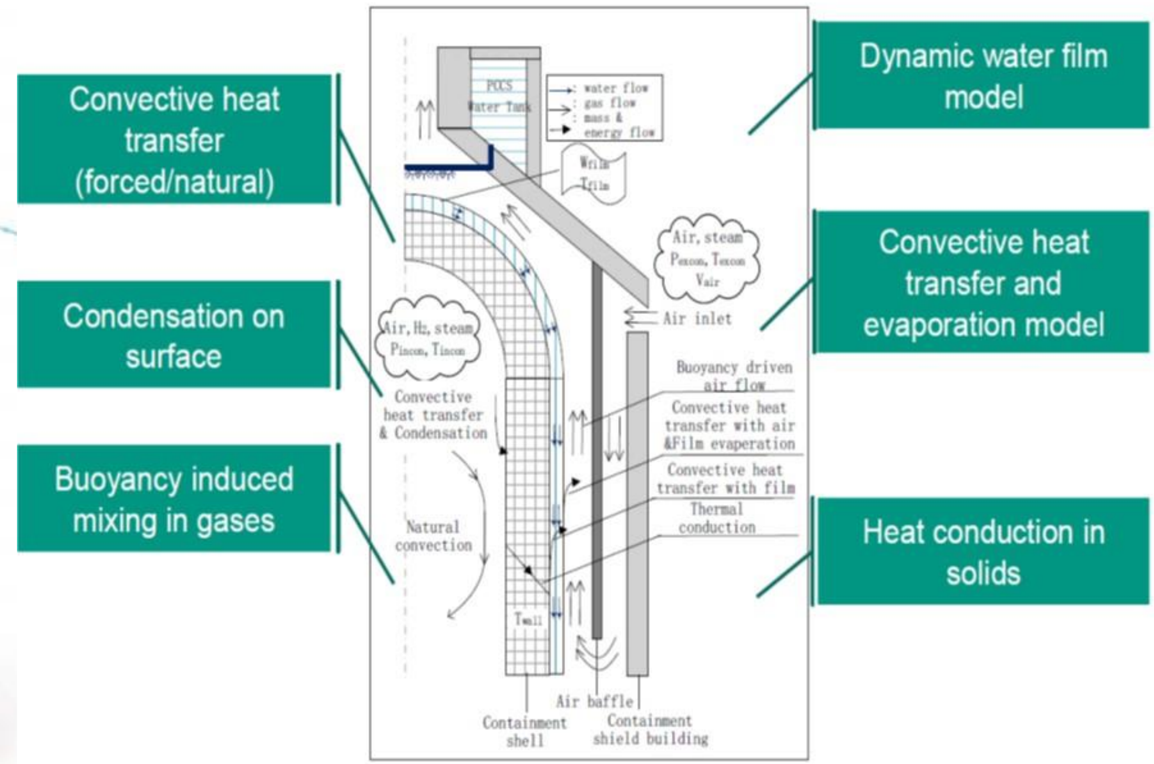


GASFLOW-MPI



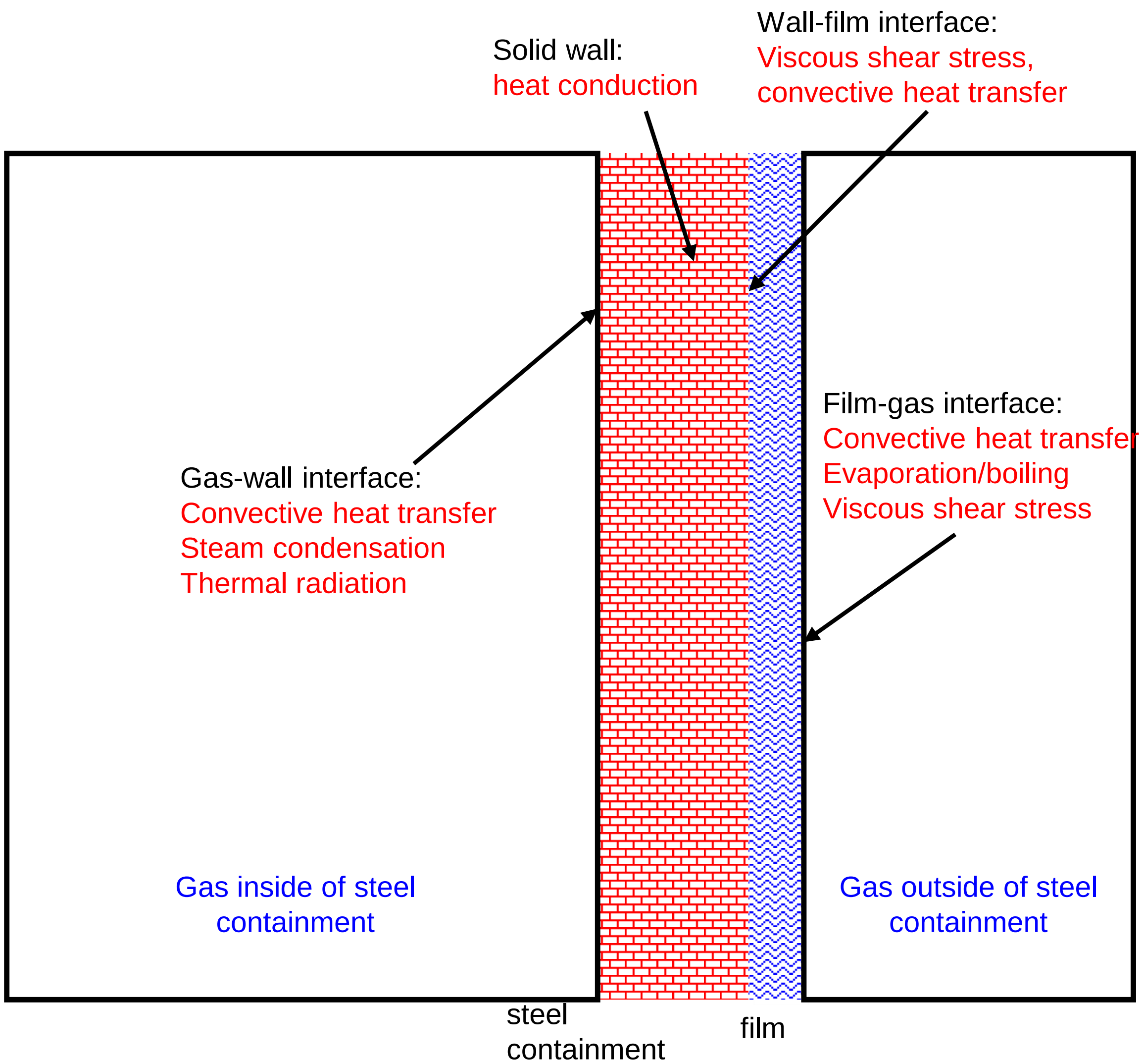
J. Xiao, J. R Travis, M. Kuznetsov: “Numerical Investigations of Heat Losses to Confinement Structures from Hydrogen-Air Turbulent Flames in ENACCEF Facility”. International Journal of Hydrogen Energy 09/2015; 40(38):13106–13120.

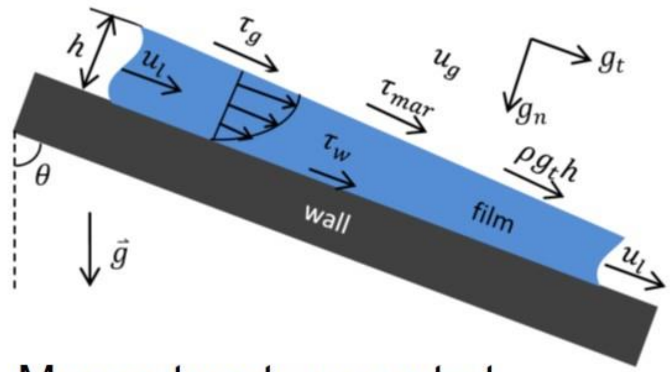
GASFLOW-MPI: Water Film Modelling
Outer Film Model for Passive Containment Cooling System



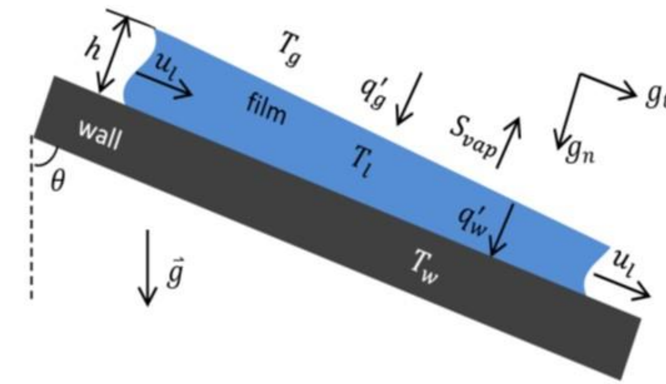
Example: Passive Containment Cooling System of AP1000

GASFLOW-MPI: Physics of liquid thin film transport



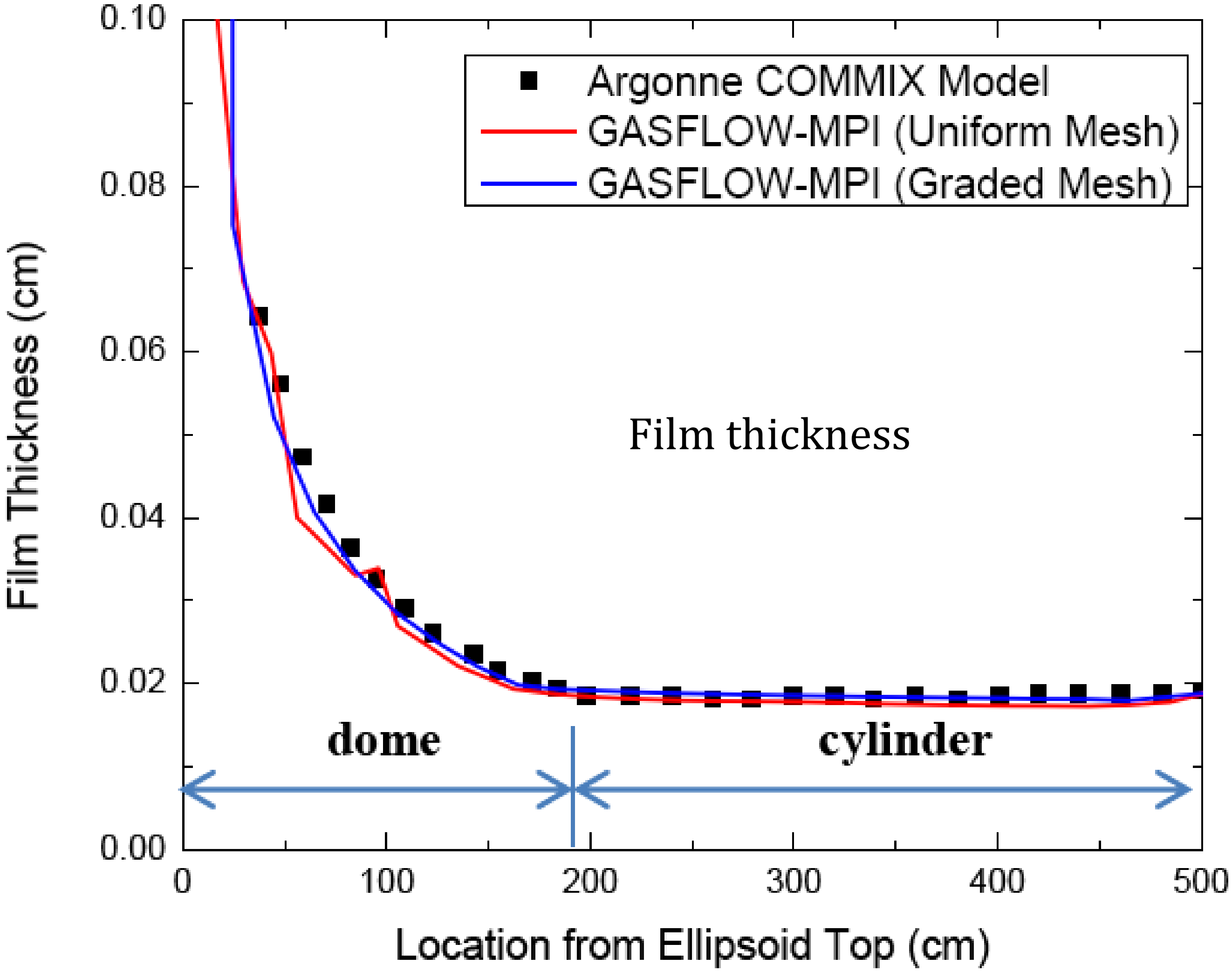


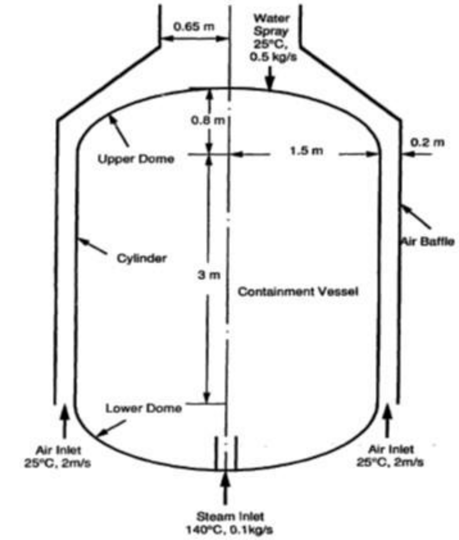
Momentum transport at interfaces of gas-film + film-wall

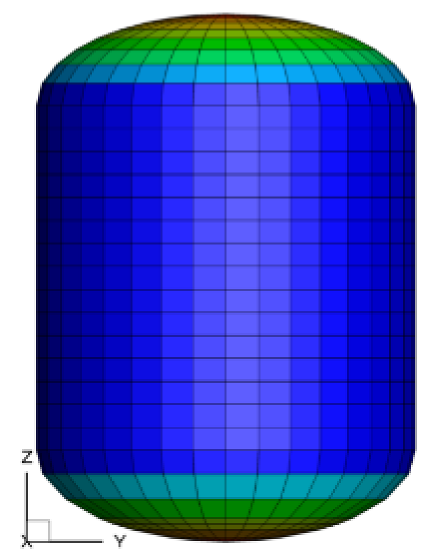


Energy transfer at interfaces of gas-film + film-wall

GASFLOW-MPI: Validation of outer film model with COMMIX Experiments







GASFLOW-MPI: Heat, Mass and Momentum Transfer at Condensation Film

- Chilton-Colburn empirical analogy

$$C_f = StPr^{2/3} = St_m Sc^{2/3} \quad 0.6 < Pr < 60; \; 0.6 < Sc < 3000$$

$$St_m = \frac{h_\mathrm{d}}{u_g} = \frac{Sh}{ReSc} \qquad Sc = \frac{\nu}{D_{AB}} \qquad Sh = \frac{h_\mathrm{d} L}{D_{AB}}$$

$$h_d = \frac{h_w}{\rho c_p} \frac{Sc^{-\frac{2}{3}}}{Pr^{-\frac{2}{3}}}$$

- and the condensation rate is calculated as:

$$\dot{m}_s = h_d^* A_w \left(\rho - \rho_{s,sat}\right)$$

$$\rho_{sat} = \frac{P_{sat}}{R_{h20} T_w}, P_{sat} = \exp\left[\frac{A(T - T_0)}{T + C}\right]$$

GASFLOW-MPI: Non-condensable Gas Absorption in Condensate Film

- The fraction of non-condensable gases in the film $n_{c,film}$:

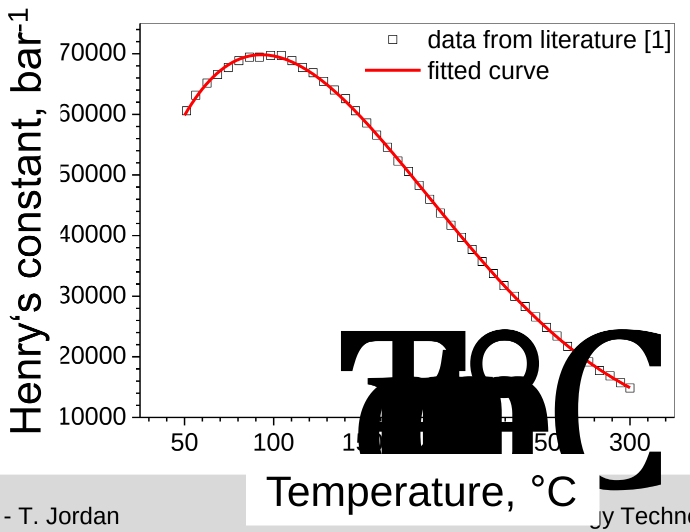
$$n_{c,film} = \frac{P_c}{H_c}, c = O_2 \; or \; H_2$$

- The static liquid film :
  - the film on the condense structure are with constant thickness δ_{min}
  - the mass and energy of the film is removed from the control volume when $\int \dot{m}_s dt \,/A_{film} > \delta_{min}$;
  - Along with the gases dissolved in the film:

$$\omega_{c,film} = \omega_{c,g} \frac{P_{gas}}{H_c} \frac{M_{gas}}{M_{film.i}}$$

$$\dot{m}_{a,c} = \omega_{c,film} \dot{m}_s$$

Where: H_c is henry constant, *c* is for components, H2 or O2; ω_c is the mass fraction, $\dot{m}_{a,c}$ is the absorption rate for component *c*



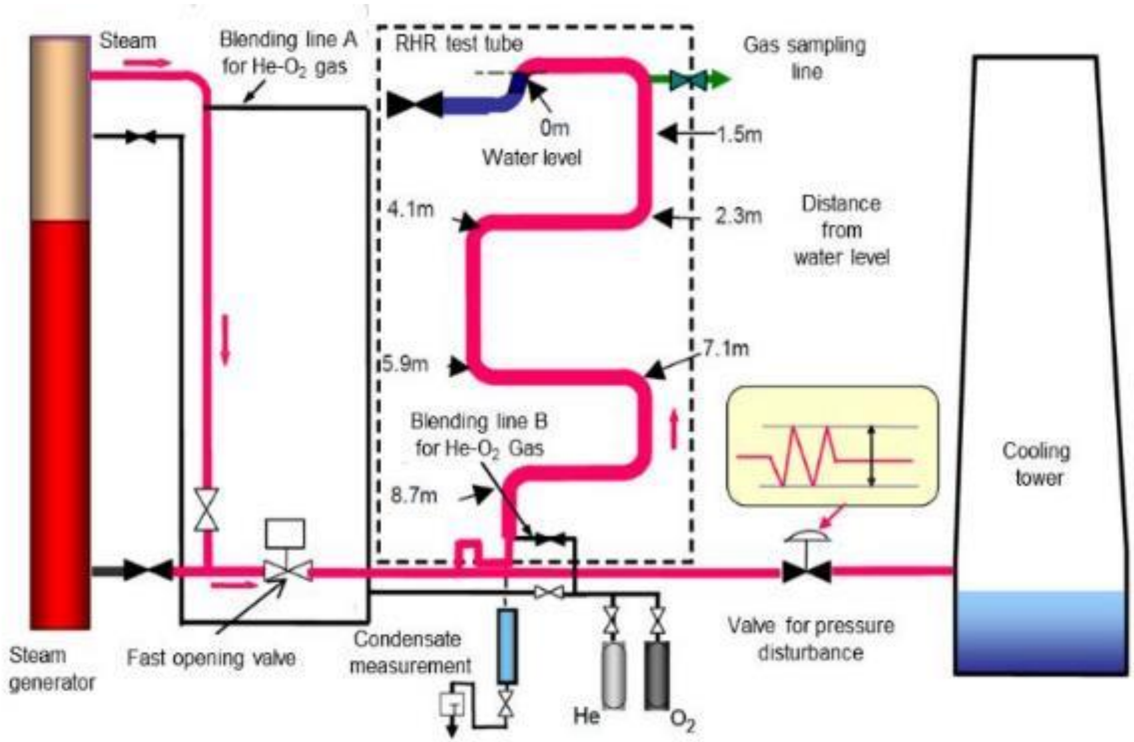
GASFLOW-MPI: Radiolytic Gas Transport Validation on the Hamaoka Pipe Experiments

Initional and boundary conditions:

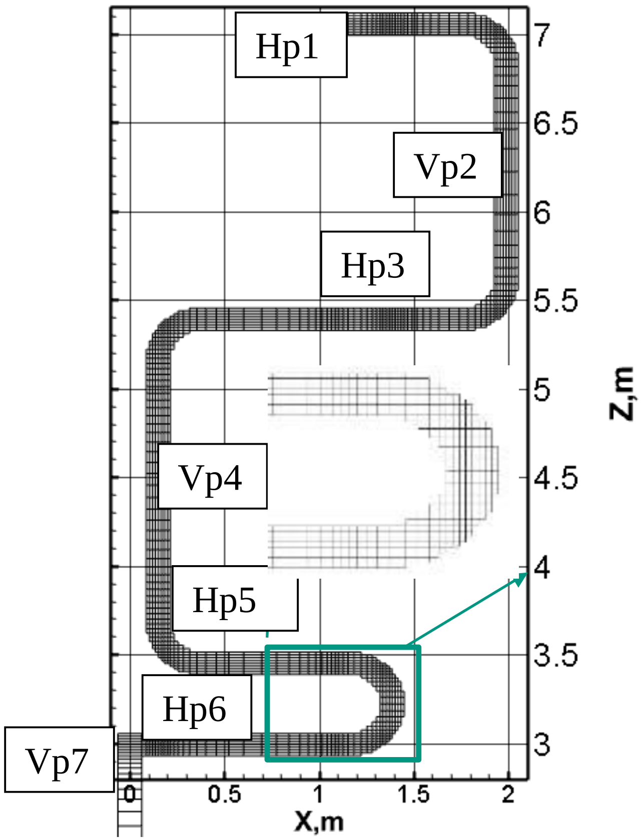
constant p=7MPa, T=286°C

$\omega_{H2,g}$ = 0.002 $\omega_{H2,g}$ = 0.016 (mole ration 2:1)

Insulator: calcium silicate wool d=65mm



Test facility for measuring enrichment of non-condensable gases (He/O_2) in the Hamaoka pipe

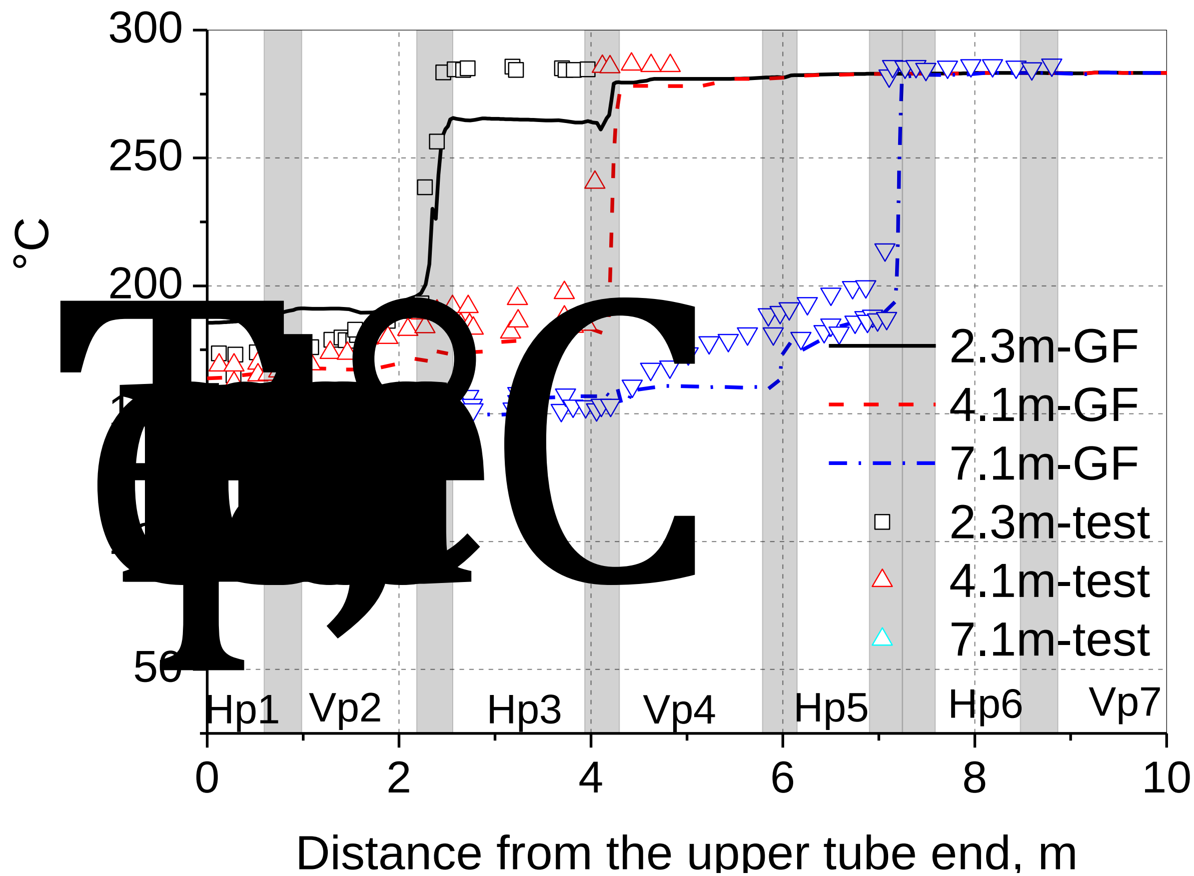


Mesh: computational domain 2.5 *1.35*7.13m in x, y and z divided 70*8*168 cells

Uniform mesh at pipe cross-section

GASFLOW-MPI: Radiolytic Gas Transport Validation on the Hamaoka Pipe Experiments

Temperature profiles associated with the distance from the upper tube end
GASFLOW-MPI (GF) versus test



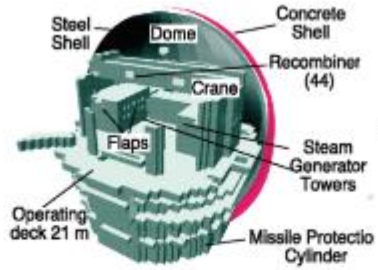
Mole fraction at Hp1

	Test	GF
Hydrogen	64.7%	63.3%
Oxygen	35.3%	31.7%

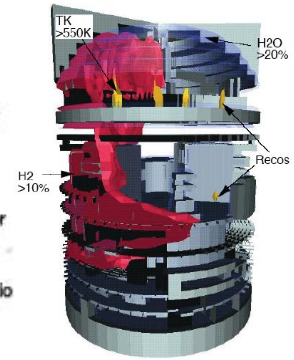
GASFLOW-MPI: Applications in Real Scale Containments

BWR

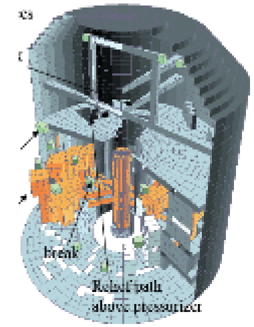
KKN



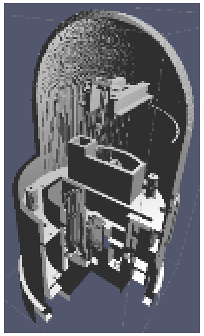
GKN



EPR

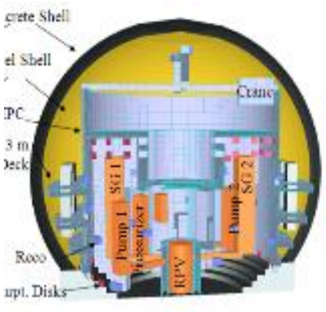


VVER

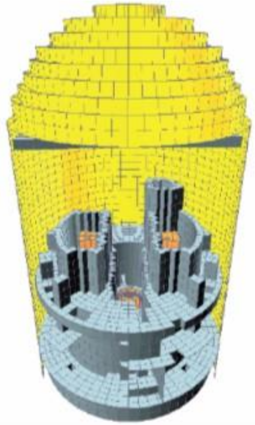


KKB

AP1000

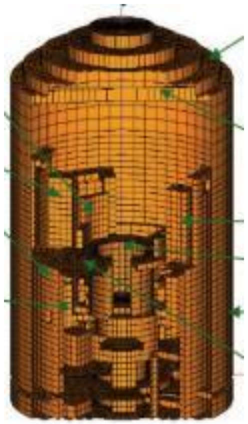


KCB

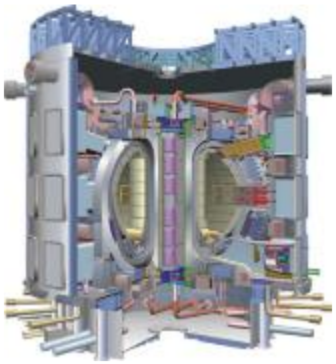


APR1400

OPR1000



Qinshan



ITER

Analytical Codes

COM3D

COM3D: Reactive Flow Modelling

- Since 1995 developed for turbulent combustion in industry relevant scales

  - 1st and 2nd exakt schemes
  - Runge-Kutta 4-order
  - Pade 6-order
  - ALE scheme for slow combustion
  - SIMPLE(…) scheme for slow combustion

- Turbulence models

  - Standard k-ε
  - RNG k-ε
  - SST k-ε & k-ω
  - LES Smagorinski, mixed, dynamic

- Thermodynamics

  - Piecewise linear approximation of JANAF tables

- Combustion models

  - Integral combustion model KYLCOM
  - +extensions: quenching, instabilities, DDT, …
  - Phenomenological models: EBU, EDC, …
  - Detonation
  - Detailed chemistry

- Special

  - Combustible dust model
  - Moving wall boundary conditions (soft wall, fragmentation,..)
  - Co-Simulation with ABAQUS

- Cutting-edge, scalable and powerful high performance computing capabilities

  - C++ skeleton with C, FORTRAN routines
  - C++ library for domain decomposition
  - MPP on basis of MPI (openMPI,..)
  - Platforms: Linux clusters; Cray, IBM (SP3, RISC)

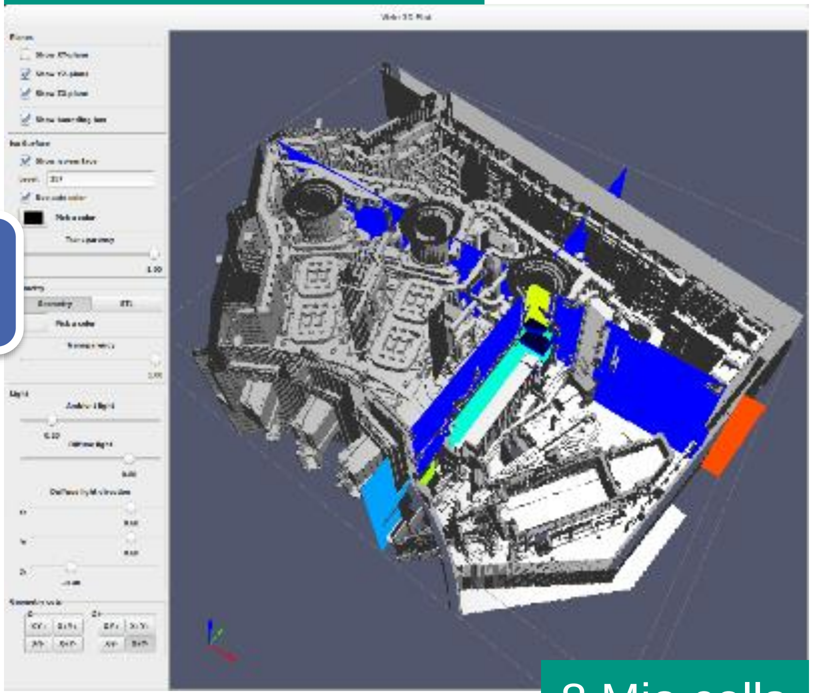
available | Under development | plan

COM3D: Process Control, Pre-, Post-Processing

Karlsruhe Institute of Technology

- Meshing
  - Structured cubic
  - Optimized Load Balancer
  - AMR
  - Immersed 3D Boundaries
- Pre-Processing
  - CAD data import
  - comgen
  - Import of GASFLOW data via comcon
- Post-Processing
  - GTK+ 3 based GUI VIZIR (incl. on-line mode)
  - Interfaces to all relevant visualization tools
- Process Control
  - Client-Server via SUN RPC
  - HDF5 data storage format

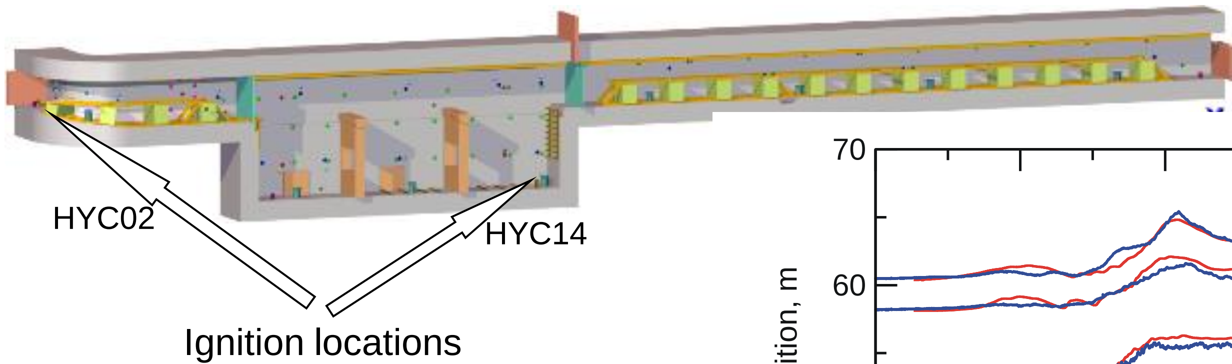
ITER NBI/Cryopump



8 Mio cells

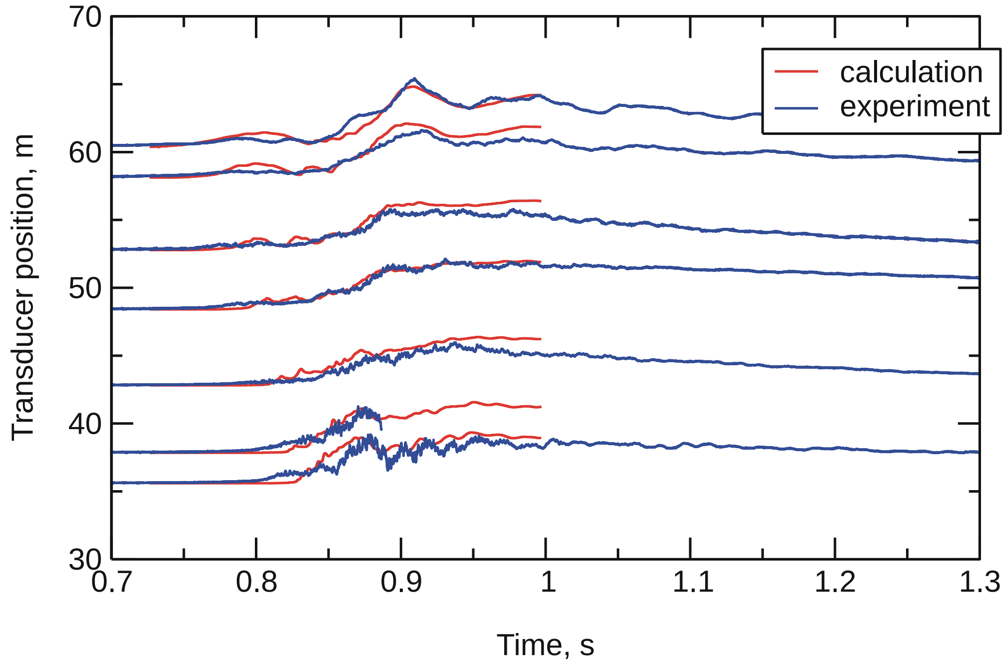
available | Under development | plan

COM3D: Typical validation
2 blind large-scale RUT facility simulations



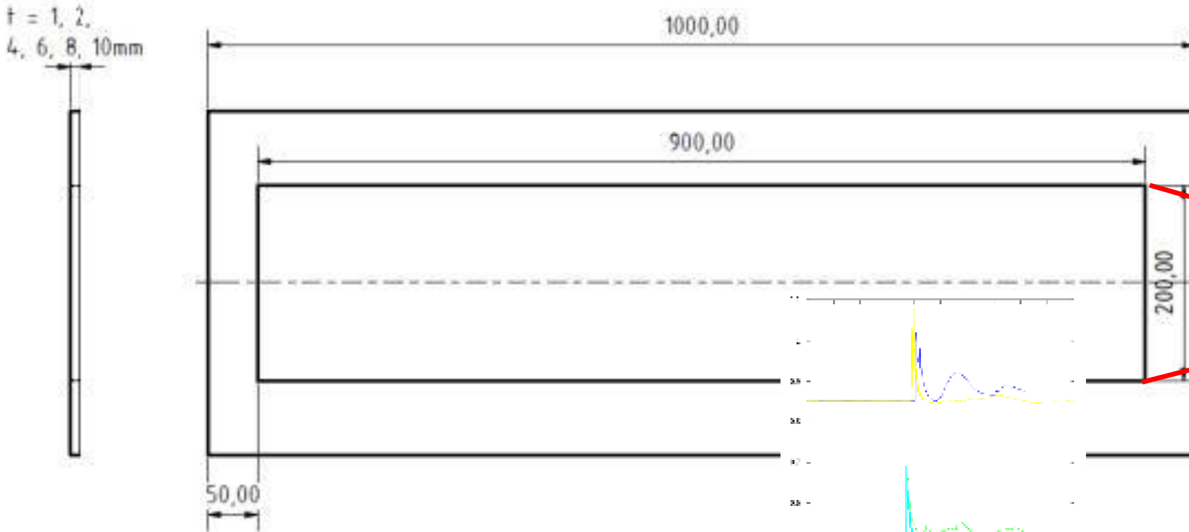
Numerical details
- Grid 98 × 94 × 416 = 3 800 000 cells
- Cells 6.67 × 6.67 × 6.67 cm
- Process time 0.27 s, 2.4 s
- 80 CPUs with total time ~20000 hours

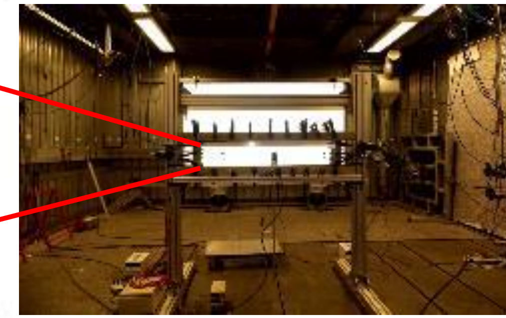
Initial conditions
- Uniformly mixed H_2 / air (11.5% vol.)
- Ignition: channel end, canyon
- P = 1 atm, T = 288 K



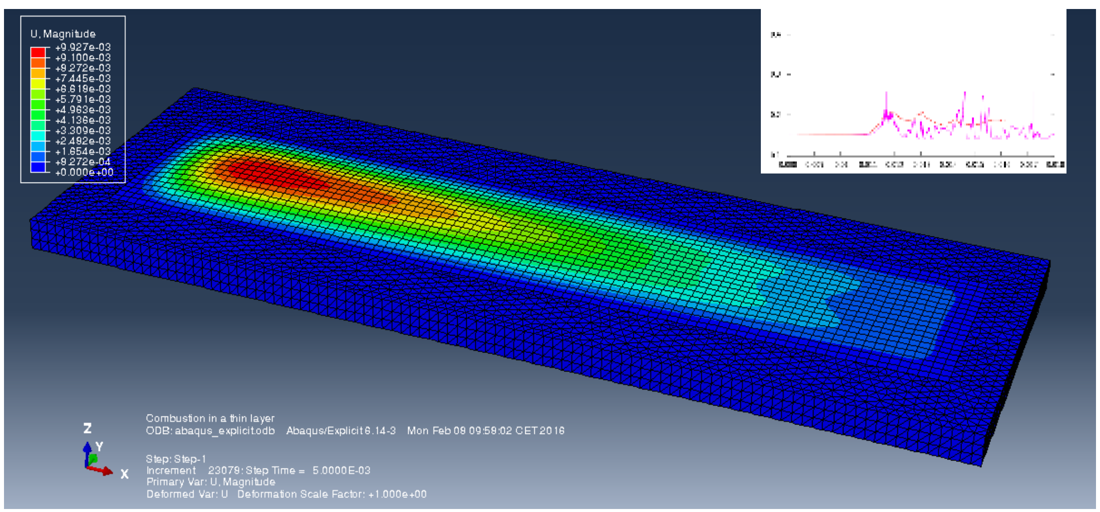
Excellent reproduction of pressure wave evolution in both blind simulations HYC02 and HYC14: Shown pressure recordings in test HYC02; transducers are located in channel and in upper part of the facility

COM3D: Fluid-Structure-Interaction Deflagration in flat channel with flexible wall



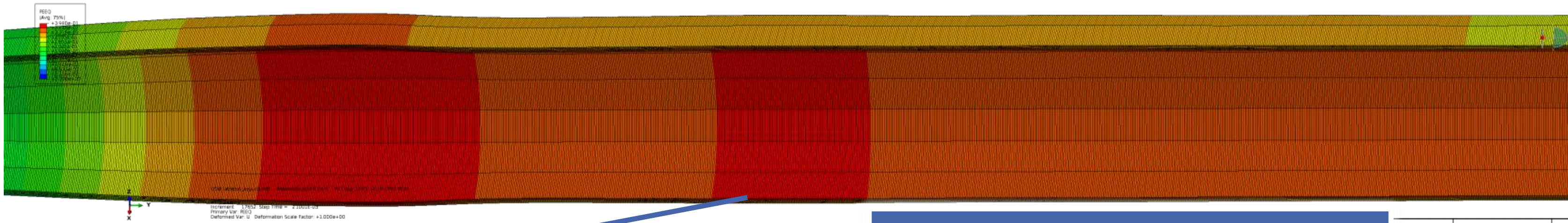


Corresponding experiment with plexiglass walls set up in HYKA Q160

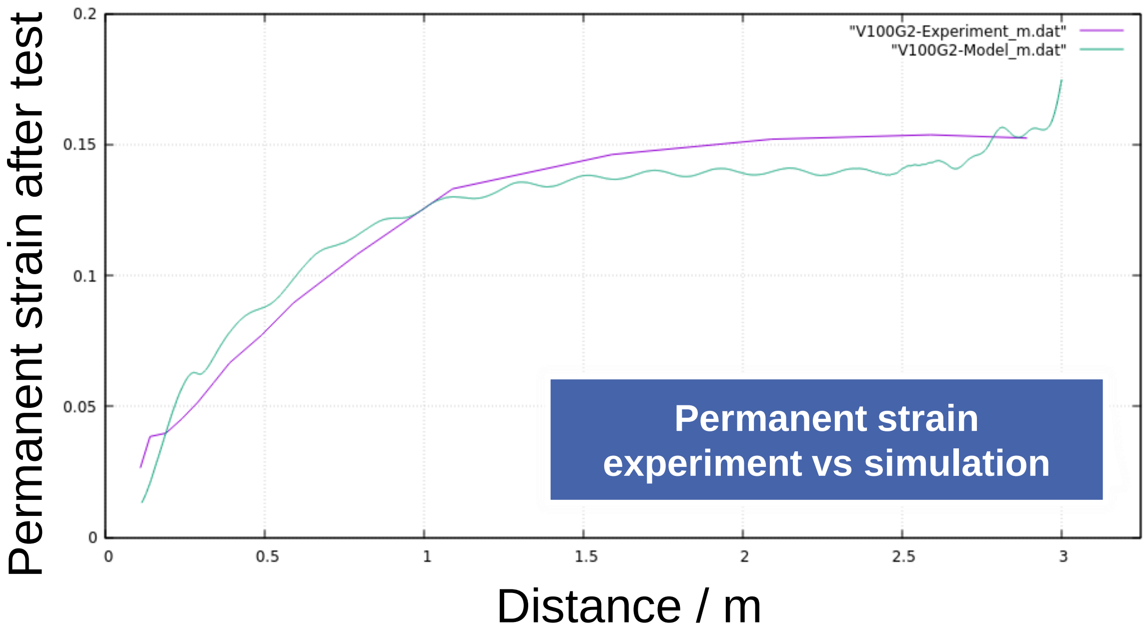


Wall displacement at t = 5 ms determined with COM3D-ABAQUS coupled calculation (co-simulation interface) applying KYLCOM+ combustion model (supported by Toyota Tsusho Europe S.A.)

COM3D: Pipeline deformation and failure behavior under detonation loads

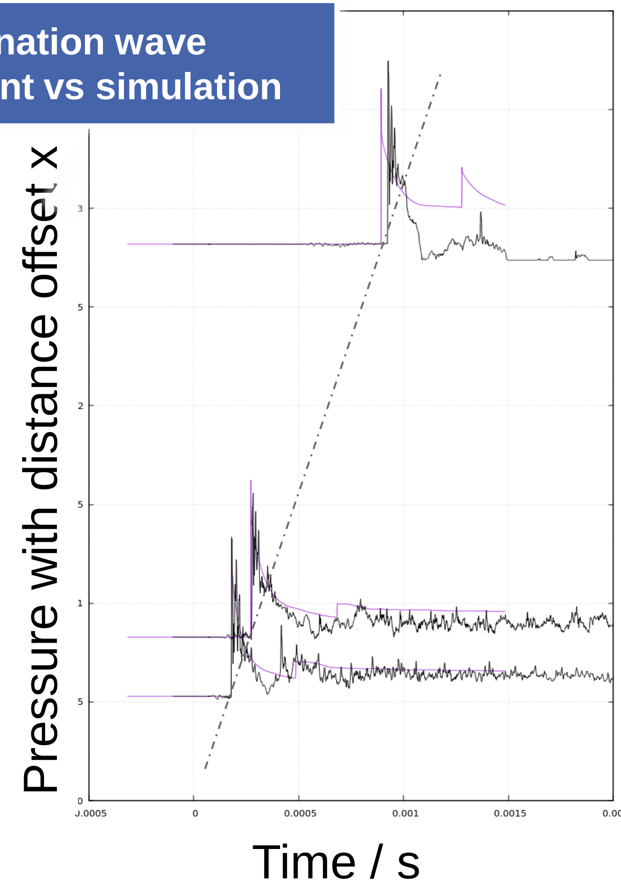


Strain Visualization

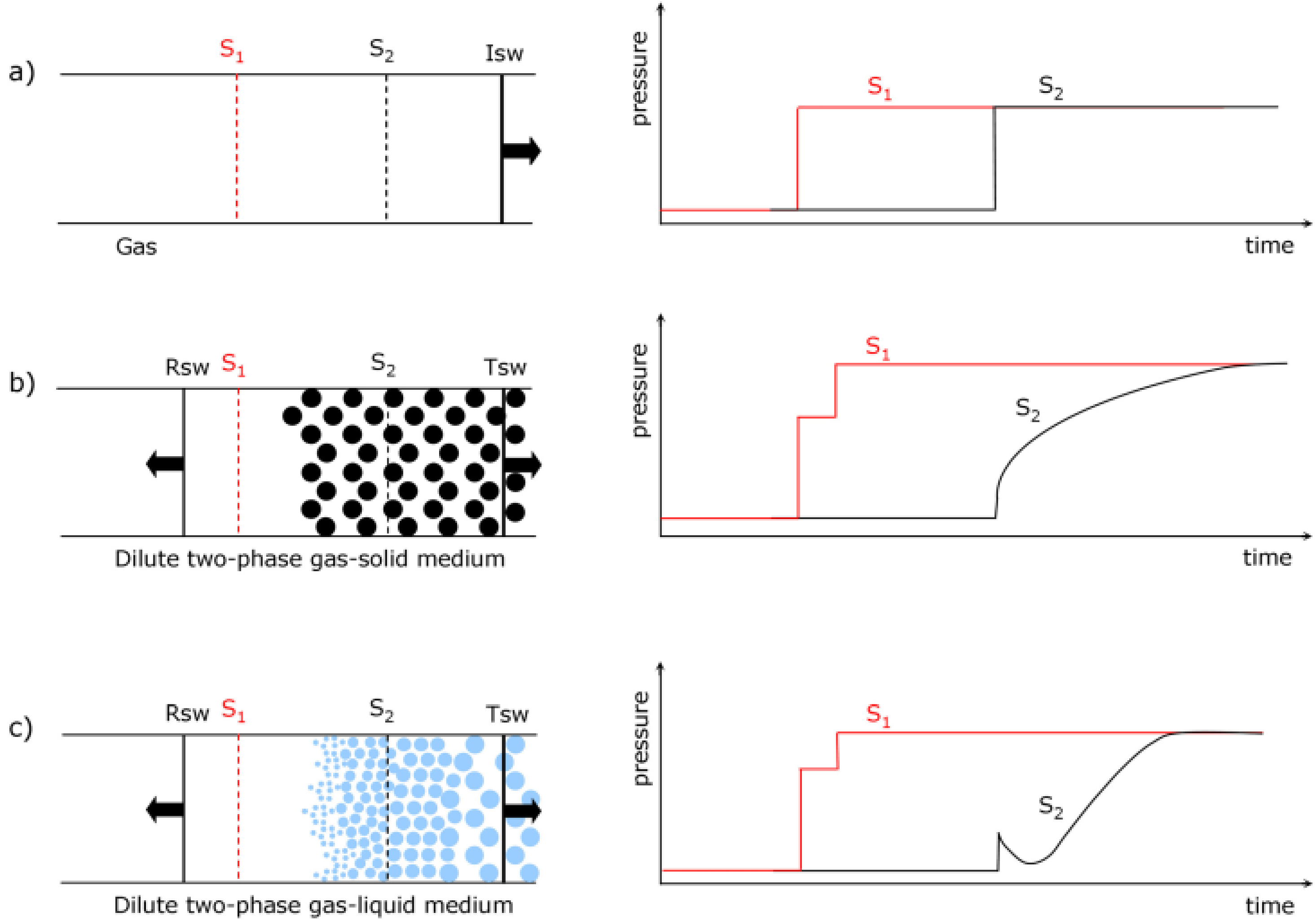


Permanent strain experiment vs simulation

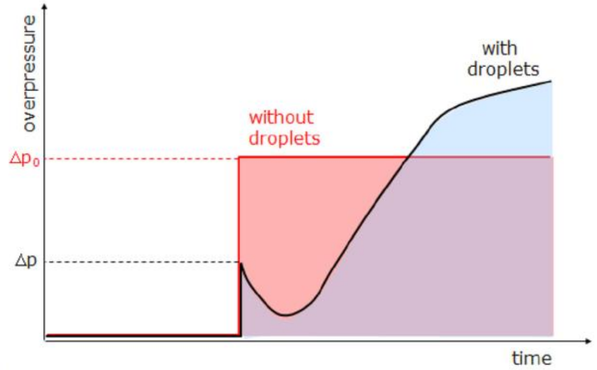
Detonation wave experiment vs simulation



COM3D: Mitigation of detonation / SW impact



COM3D: Droplet – flow interaction model



Two-way coupling of particle – flow interaction is available
Particle disintegration model is under development

- Disintegration time correlation of Pilch

$$\frac{t_b}{t^*} = \begin{cases} 6\,(\mathrm{We}-12)^{-0.25} & 12 < \mathrm{We} < 18 \\ 2.45\,(\mathrm{We}-12)^{0.25} & 18 < \mathrm{We} < 45 \\ 14.1\,(\mathrm{We}-12)^{-0.25} & 45 < \mathrm{We} < 351 \end{cases}$$

- Corrected We-number for On > 0.1:

$$\mathrm{We}_{corr} = \frac{\mathrm{We}}{1\,+\,1.077\,\mathrm{On}^{1.6}}$$

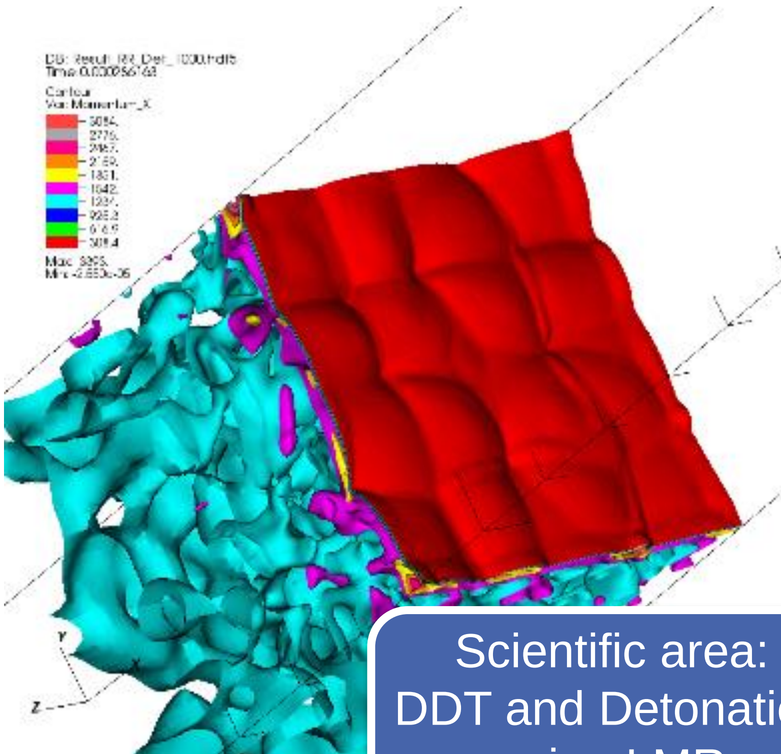
- Correlation for secondary droplet sizes

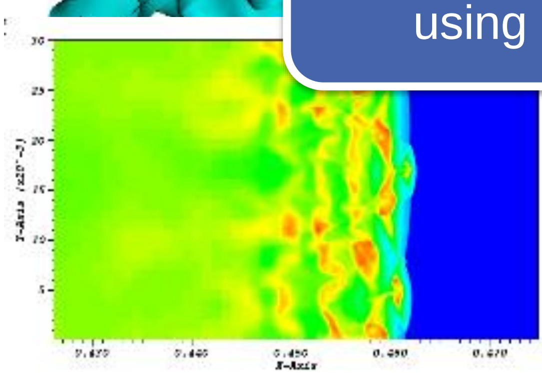
$$\frac{D_{32}}{D_0} = 1.5\,\mathrm{On}^{0.2}\,\mathrm{We}_{corr}^{-0.25}$$

- Correlation for droplet size distribution

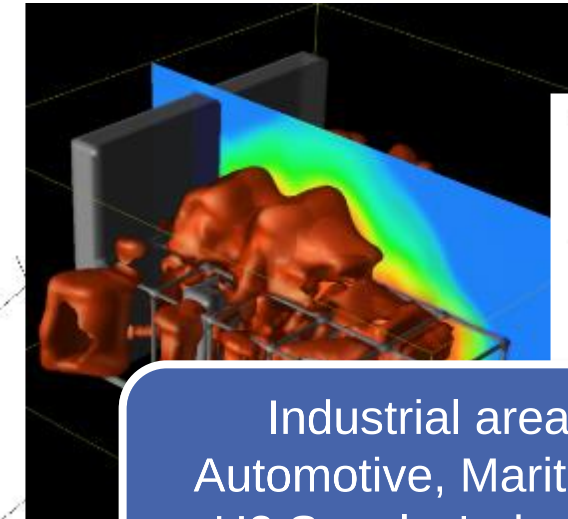
$$f(D) = \frac{x}{2\sqrt{2\pi}\,\sigma\,D}\,\exp\left\{-\frac{1}{2}\left[\frac{x\,-\,\mu}{\sigma}\right]^2\right\}$$

COM3D: Application Areas

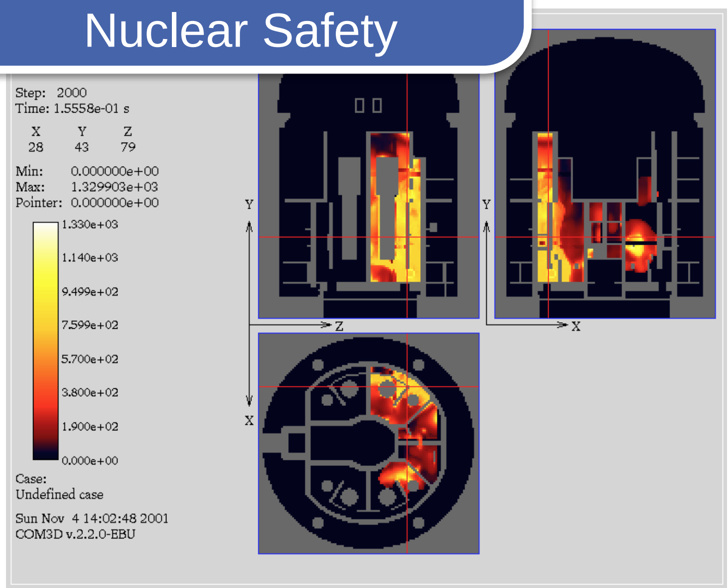




Scientific area:
DDT and Detonation
using LMR



Industrial area:
Automotive, Maritime,
H2 Supply, Industry,
Nuclear Safety



CLOSURE

User Community and Licensing

GASFLOW-MPI User Community

~ 25 licenses worldwide
(5 Germany, 12 China, 2 South Korea,
2 Mexico, 2 France, 1 Hungary and
1 Czech Republic)

Strong, expanding position in nuclear community

COM3D User Community

Research focused, universities, testing of combustion models

License Models

- GASFLOW-MPI: commercial, with services, application focused
- COM3D: research & education; open (free) source

Outlook

GASFLOW-MPI and COM3D

More applications also in the non-nuclear field, e.g. hydrogen supply infrastructure, fuel cells, vehicles, maritime, aviation, space, etc.

GASFLOW-MPI

- Special commercial services, in particular for Asia (spin-off in China)
- Improved user interfaces
- Further acceleration via domain decomposition, GPUs, etc
- Stochastic spray model, porous media, multi-phase H2, particle model,…

COM3D

- Immersed boundaries (moving walls)
- Co-simulation interface
- Shockwave- and flame-water spray interaction