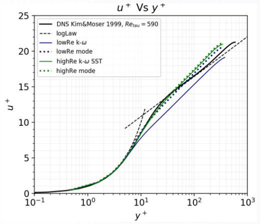
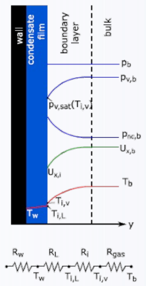
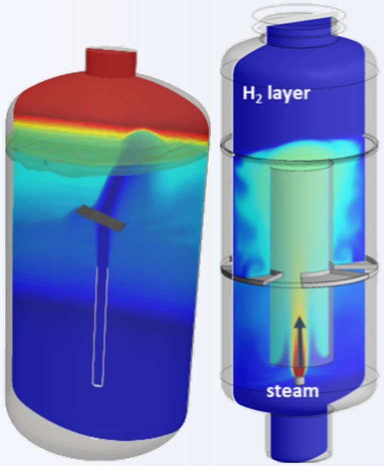
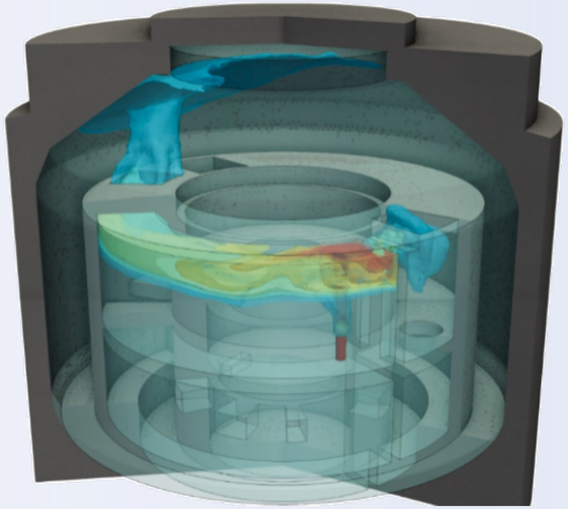
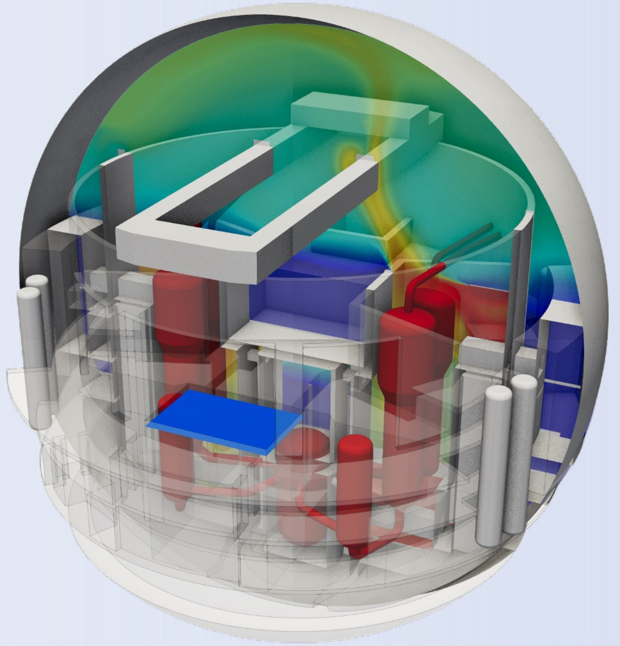




$$\frac{\partial(\rho\vec{U})}{\partial t} + \nabla\cdot(\rho\vec{U}\otimes\vec{U}) = -\nabla p + \nabla\cdot\tau + \rho\vec{g}$$







Introduction to *containmentFOAM*

S. Kelm

Joint ICTP-IAEA Workshop on Open-Source Nuclear Codes for Reactor Analysis, ICTP Trieste, Italy, Aug 7th-11th 2023

The Abdus Salam International Centre for Theoretical Physics

IAEA International Atomic Energy Agency

Supported by:

Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection

based on a decision of the German Bundestag

Project No. 150 1633B

containment∇FOAM

JÜLICH Forschungszentrum

Mitglied der Helmholtz-Gemeinschaft

ACKNOWLEDGEMENTS (1)

JÜLICH Forschungszentrum

The developers and maintainers team

containmentFOAM Contributors:

- Stephan KELM (Principal Investigator) 2015 -
- Manohar KAMPILI (Turbulence, Aerosols, Maintenance) 2015 -
- Vijaya Kumar GOPALA KRISHNA MOORTHY (Multispecies, Wall Condensation, Turbulence, Aerosols) 2016 -
- Astrid KUHR (Maintenance, Repository) 2016 -
- Xiongguo LIU (Thermal Radiation, REKODIREKT Coupling) 2017 -
- Markus HORRMANN (REKODIREKT Coupling) 03/2019 - 11/2019
- Kinshiro SAKAMOTO (Wall Condensation) 08/2018 - 2/2019
- Claudia DRUSKA (REKODIREKT development, general validation) 2018 -
- Stephan STRUTH (REKODIREKT development) 2019 -
- Daniel SCHUMACHER (GUI development, Solver Monitor, adaptive time stepping) - 02/2019 -
- Liam M.F. CAMMIADE (Wall Condensation) 2019 -
- Ruiyun JI (Uncertainty Quantification) 2019 -
- Allen GEORGE (Bulk Condensation) 2020 -
- Lucian RADEMACHER (GUI development) 2020 - 2022
- Leon Thelen (GUI development) 2022 -
- Karl STURM (systemCoupling, FMI interface) 10/2022 -

ACKNOWLEDGEMENTS (2)

JÜLICH Forschungszentrum

Sponsors and Projects

- German Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection (BMUV) for funding code maintenance and integration to the national CFD reference package CF2REF (Fkz **150 1633B**) as well as the ongoing projects UQ4CFD (Fkz **150 1595**) and SETCOM-2 on wall condensation modeling (Fkz **150 1591**)
- Former German Federal Ministry of Economic Affairs and Energy (BMWi) and for funding projects related to further development of CFD for reactor safety application (Fkz **150 1407)** and the REKO experimental and model development program (Fkz **150 1308 / 150 1394 / 150 1470**) as well as the SETCOM projects (Fkz **1501404 / 1501489**)
- Becker Technologies GmbH for carefully conducting, documenting and sharing the experimental data of the national THAI programs, in particular the experiments TH2 (THAI-1, BMWi Fkz **1501218**), TH24.3 (THAI-3, BMWi Fkz **1501361**) and TH32 (THAI-VI, BMWi Fkz. **1501594**)
- **H**elmholtz **I**nterdisciplinary Doctoral **T**raining in **E**nergy and **C**limate Research (HITEC) Graduate School, the German Academic Exchange Service (DAAD) and the Chinese Scholarship Council (CSC) for funding PhD positions and student exchange
- **IAEA O**pen-source **N**uclear **CO**des for **RE**actor Analysis (**ONCORE**) initiative, a collaborative framework for the development and application of open-source multiphysics to support research, education, and training in analysis of advanced reactor designs

Supported by: Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection

based on a decision of the German Bundestag

Supported by: Federal Ministry for Economic Affairs and Climate Action

on the basis of a decision by the German Bundestag

BECKER TECHNOLOGIES

HiTEC Graduate School for energy & climate

Bundesministerium für Bildung und Forschung

DAAD

CHINA SCHOLARSHIP COUNCIL

IAEA International Atomic Energy Agency

ACKNOWLEDGEMENTS (3)

JÜLICH
Forschungszentrum

Partners

- Prof. K. Arul Prakash (Indian Institute of Technology Madras) for collaborating under IITM-RWTH Joint Doctoral Program, DAAD IIT-MSP Programs.
- Dr. Berthold Schramm and Dr. Jörn Stewering (GRS) for their collaboration within the CF2REF project
- Prof. Markus Klein (Universität der Bundeswehr München), Prof. Xu Cheng (Karlsruhe Institute of Technology) and Prof. Reinhold Kneer (RWHT Aachen University) for supervising the involved PhD students and their collaboration within the UQ4CFD and SETCOM-2 projects.
- Our contributors, partners and colleagues and beta testers

And not to forget:

- The original developers, maintainers an contributors of OpenFOAM® !

GRS global research for safety

Universität der Bundeswehr München

KIT Karlsruhe Institute of Technology

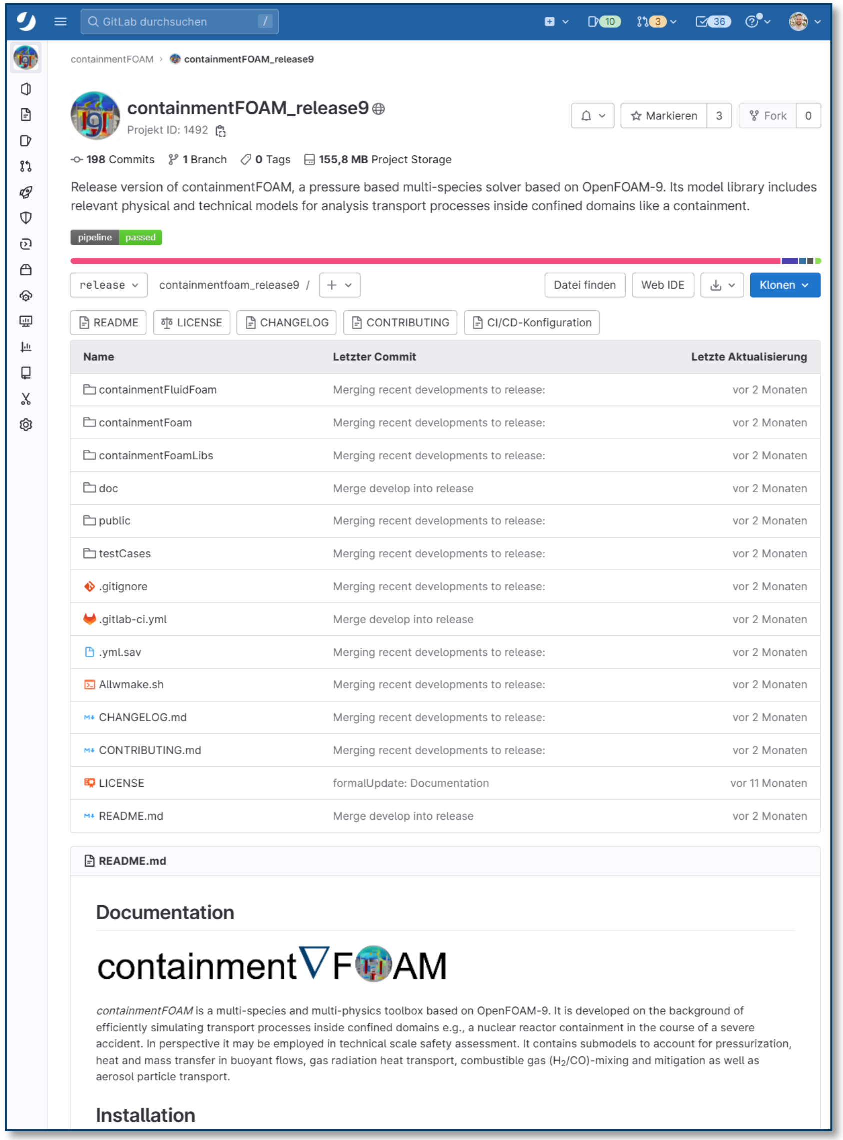
WSA Institute of Heat and Mass Transfer | RWTH AACHEN UNIVERSITY

CFD

Open∇FOAM®

OpenFOAM The OpenFOAM Foundation

- Public containmentFOAM repository
  https://go.fzj.de/containmentFOAM



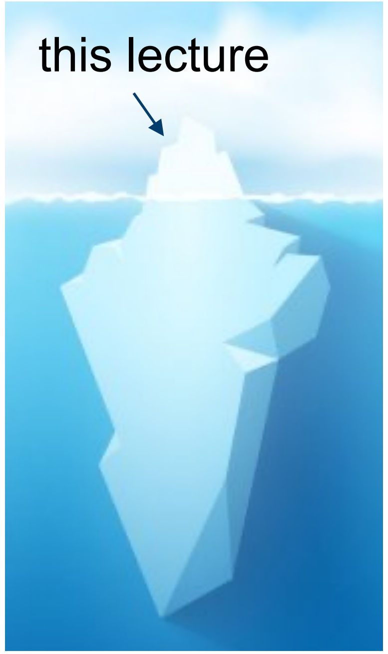
OBJECTIVES OF THIS LECTURE

- give an example of how to tailor OpenFOAM for a nuclear safety application
  - what is containment∇FOAM
  - ..and what are its target applications ?

  we'll discuss a bit about
  Severe Accidents & containment analysis

  - which functionality do we use
    - standard functionality in OF can we use
    - .. and which specialized modeling approaches do we need?
    - .. and how are they implemented ?

  we'll have a quick look
  at the models and code



https://st2.depositphotos.com/1063116/5632/v/950/depositphotos_56324557-stock-illustration-iceberg-concept-illustration.jpg

- future perspectives of containmentFOAM

OUTLINE

- Severe Accidents and Containment Analysis
- Development of containment∇FOAM
- Theoretical Background
  - Buoyancy driven turbulent multi-species flows
  - Condensation processes
  - Thermal radiation
  - System models (PARs, code coupling, burst discs, porous models)
- containment∇FOAM framework
  - repository
  - cfGUI and cfSolutionMonitor
- Summary and Conclusions

OUTLINE

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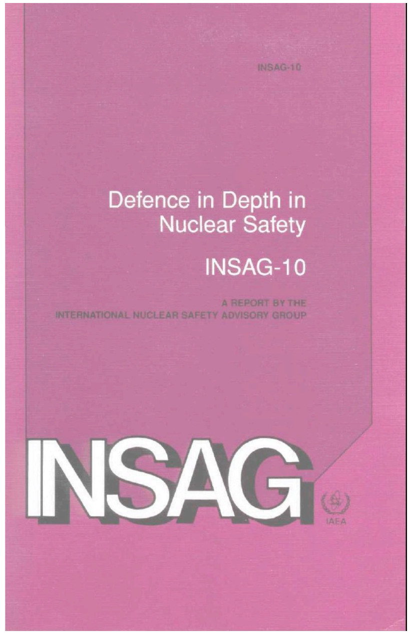
SEVERE ACCIDENTS

Defense-in-Depth Safety Concept of NPPs

- IAEA Definition (1996)
  - Concept of staggered barriers against release of fission products:
    - Fuel matrix
    - Fuel cladding
    - Reactor cooling system
    - Containment
  - Protection of the barriers by multi-level measures
  - ➢ Severe Accident: Level 4&5
    - Failure of all active systems
    - Damage of one ore more barriers (fuel matrix, cladding and RCS)
      Remaining barrier: Containment

	Levels of defence in depth	Objective	Essential means
DBA	Level 1	Prevention of abnormal operation and failures	Conservative design and high quality in construction and operation
DBA	Level 2	Control of abnormal operation and detection of failures	Control, limiting and protection systems and other surveillance features
DBA	Level 3	Control of accidents within the design basis	Engineered safety features and accident procedures
BDBA / SA	Level 4	Control of severe plant conditions, including prevention of accident progression and mitigation of the consequences of severe accidents	Complementary measures and accident management
BDBA / SA	Level 5	Mitigation of radiological consequences of significant releases of radioactive materials	Off-site emergency response

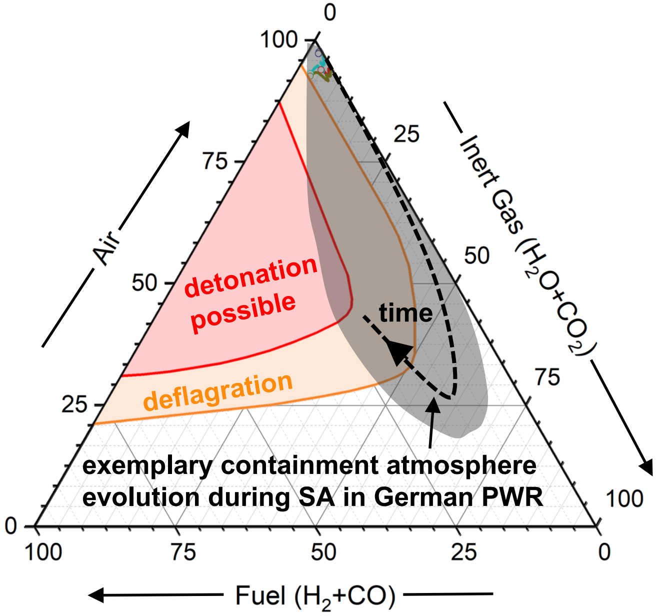


📖 https://www-pub.iaea.org/MTCD/publications/PDF/Pub1013e_web.pdf

SEVERE ACCIDENTS

Combustion Risk

- Continuous H_2 release during in-vessel and $H_2+CO+CO_2$ release during ex-vessel phase
  - Formation of flammable mixtures possible due to
    - Local accumulation or atmospheric stratification
    - Condensation / venting of steam
  - Slow combustion: $p < p_{AICC}$ (adiabatic isochoric complete combustion pressure)
    - Flame speed $O \sim 1\ cm/s$ (thermal loads)
  - Fast combustion and DDT: p may locally exceed p_{AICC}
    - Flame speed $O \sim 100\ m/s\ ..\ c$ (speed of sound)
    - Shock waves, dynamic effects (mechanical loads)
  - Standing flames:
    - Local overheating of structures (e.g. by the continuous burning of the hydrogen generated during MCCI)



Ternary diagram, own figure

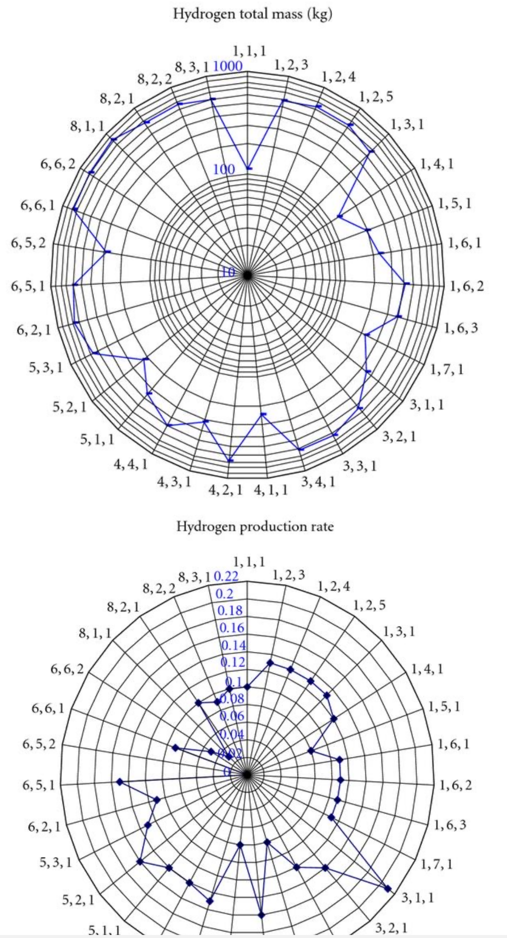
H2 explosion at F1-3

https://www.ensi.ch/de/wp-content/uploads/sites/2/2014/09/tfk1_13.png

CFD APPLICATION TO SEVERE ACCIDENTS

Analysis Chain

- CFD is mostly used as an element in a safety assessment, e.g., H_2-risk:
  - Step 1 – Selection of plant design and geometry
  - Step 2 – Selection of relevant scenarios – Probabilistic methods, fast running codes
  - Step 3 – Determination of source terms from core damage
  - Step 4 – **Analysis of gas mixing and flammable could evolution** – System codes, 3D and CFD codes (containment∇FOAM)
  - Step 5 – Assess potential of flame acceleration (or DDT) – empirical criteria
  - Step 6 – **Evaluation of pressure loads (e.g., explosionDynamicsFoam)**
  - Step 7 – **Implementation of safety measures, re-assessment (step 4-6)** or determination of structural response (FSI)



Total H_2 mass and release rate for different scenarios at a French PWR900
Figures from Bentaib et al.,2010

Adopted from:
W. Breitung, P. Royl, "Procedure and tools for deterministic analysis and control of hydrogen behavior in severe accidents", Nuclear Engineering and Design 202, 2000

A. Bentaib et al., „Evaluation of the Impact That PARs Have on the Hydrogen Risk in the Reactor Containment: Methodology and Application to PSA Level 2", Science and Technology of Nuclear Installations, 2010, 320396 https://doi.org/10.1155/2010/320396

CFD APPLICATION TO SEVERE ACCIDENTS

Experimental Database and (System) Code Validation

- CFD can fill the gaps between experiments and system code (validation)
  - Detailed understanding where measurements are impossible or difficult (e.g., rough conditions, fast transients)
    - Supporting evaluation of the experiment, design of appropriate nodalisation scheme or evaluation of closure models
  - Comparably cheap for parametric studies (DoE, Sensitivity etc.)
    - Supporting design and evaluation of application-oriented experiments, scaling
  - Virtual transfer of experiential results (scaling, interactions under realistic conditions)
  - Assessment of local / 3D effects & geometrical constraints
    - Quantification of safety margins / implications, effectiveness of passive safety systems
- Challenges:
  - Isolation of the ‘problem’ and definition of IC&BC with higher level of detail
  - Often need for ‘non-standard’ models
  - Consideration of ‘system feedback’

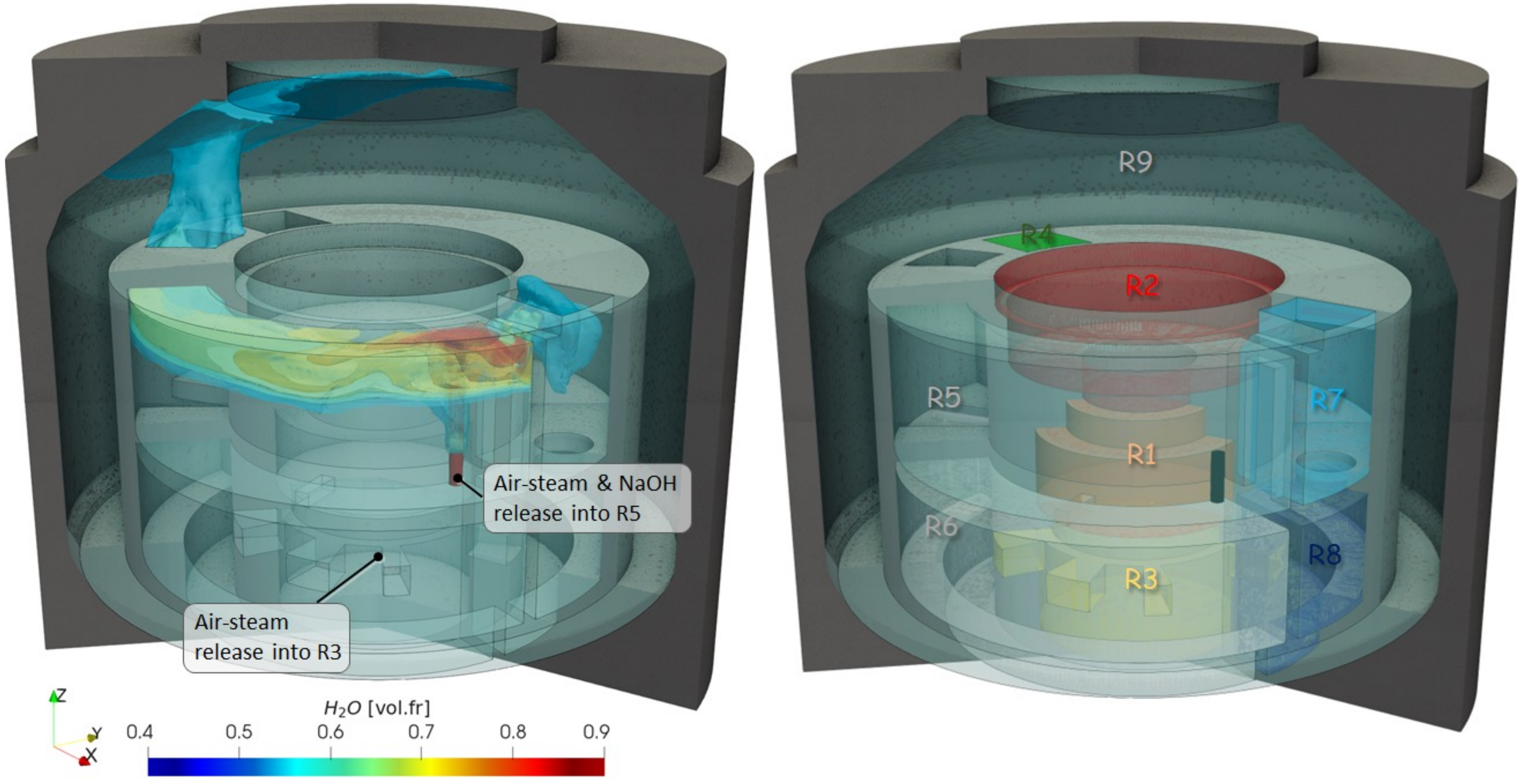
APPLICATION EXAMPLES

- Re-assessment of the ISP-37 VANAM M3 experiment in the Batelle Model Containment
- Integration in the analysis chain for combustion risk assessment in a PWR containment
- H_2 risk assessment in industrial installations
- In perspective: Application to iPWR SMR concepts safety assessment

APPLICATION EXAMPLES

ISP37 - VANAM M3 Experiment - Experimental Setup

- Multi-compartment Aerosol Depletion Test with Soluble / Hygroscopic Aerosol Material (NaOH)
  - ~626 m³ Battelle Model Containment
  - 9 compartments representing the characteristic (German) PWR containment compartmentalization
  - Concrete building without liner → leakage
  - Experimental campaign conducted in 1990's → no digital documentation
  - Integral effect tests



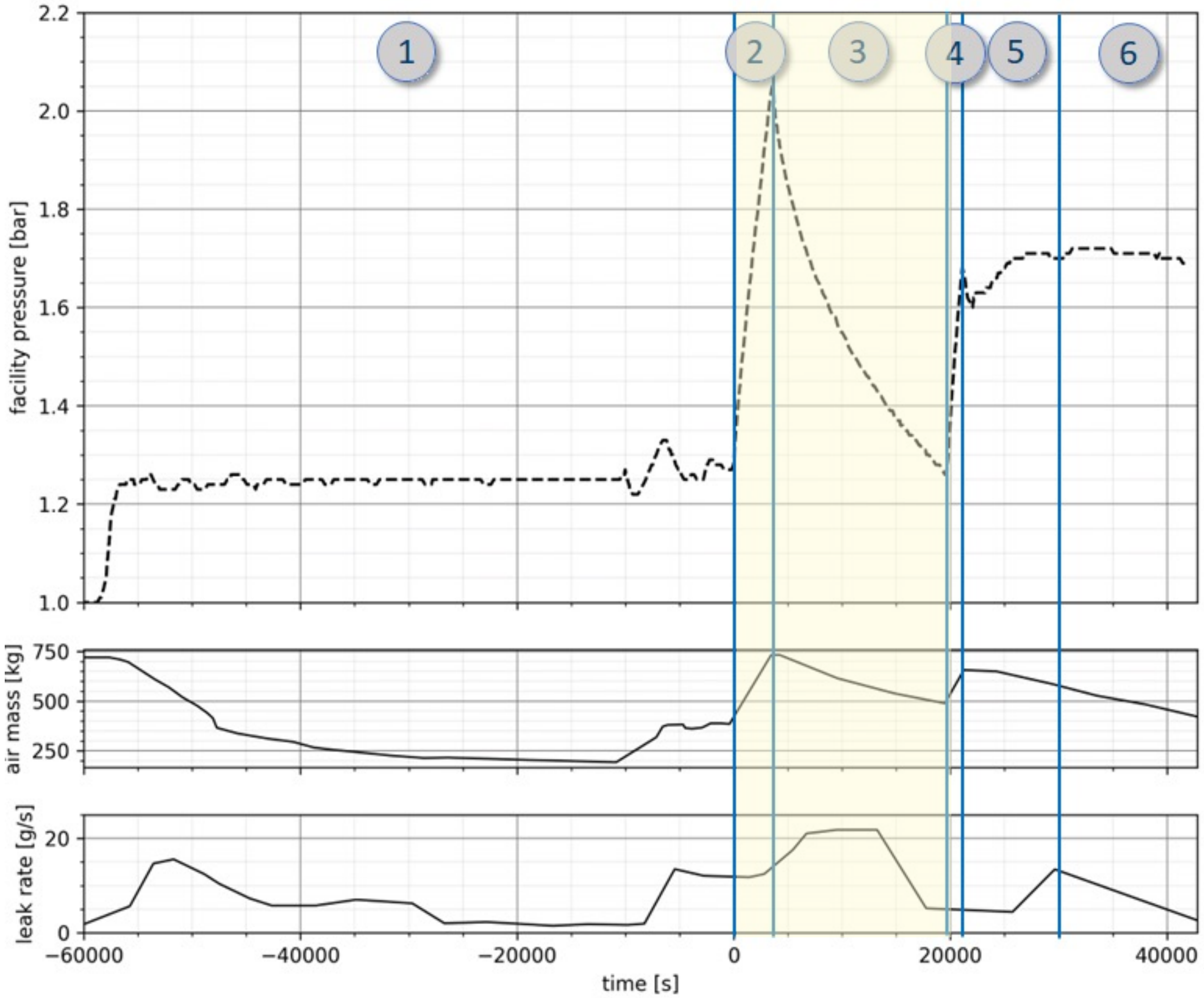
M. Firnhaber et al., „*ISP-37 – VANAM M3 A Multi Compartment Aerosol Depletion Test with Hygroscopic Aerosol Material*", NEA/CSNI/R(96)26, 1996
T. Kanzleiter, „*V ANAM Multi-compartment Aerosol Depletion Test M3 with Soluble Aerosol Material* ", Technical Report BIeV-R67.098-304, July 1993

APPLICATION EXAMPLES

ISP37 - VANAM M3 Experiment - Procedure

- Complex 30 h transient
  - phase 1: facility pre-conditioning and heat-up
  - phase 2: first NaOH aerosol injection to R5 (suspended in steam-air mixture)
  - Phase 3: aerosol depletion
  - Phase 4: second NaOH injection to R5
  - Phase 5: aerosol depletion while steam injection to R3
  - Phase 6: aerosol depletion while steam injection to R5

➢ Here application-oriented assessment based on phases 2-3



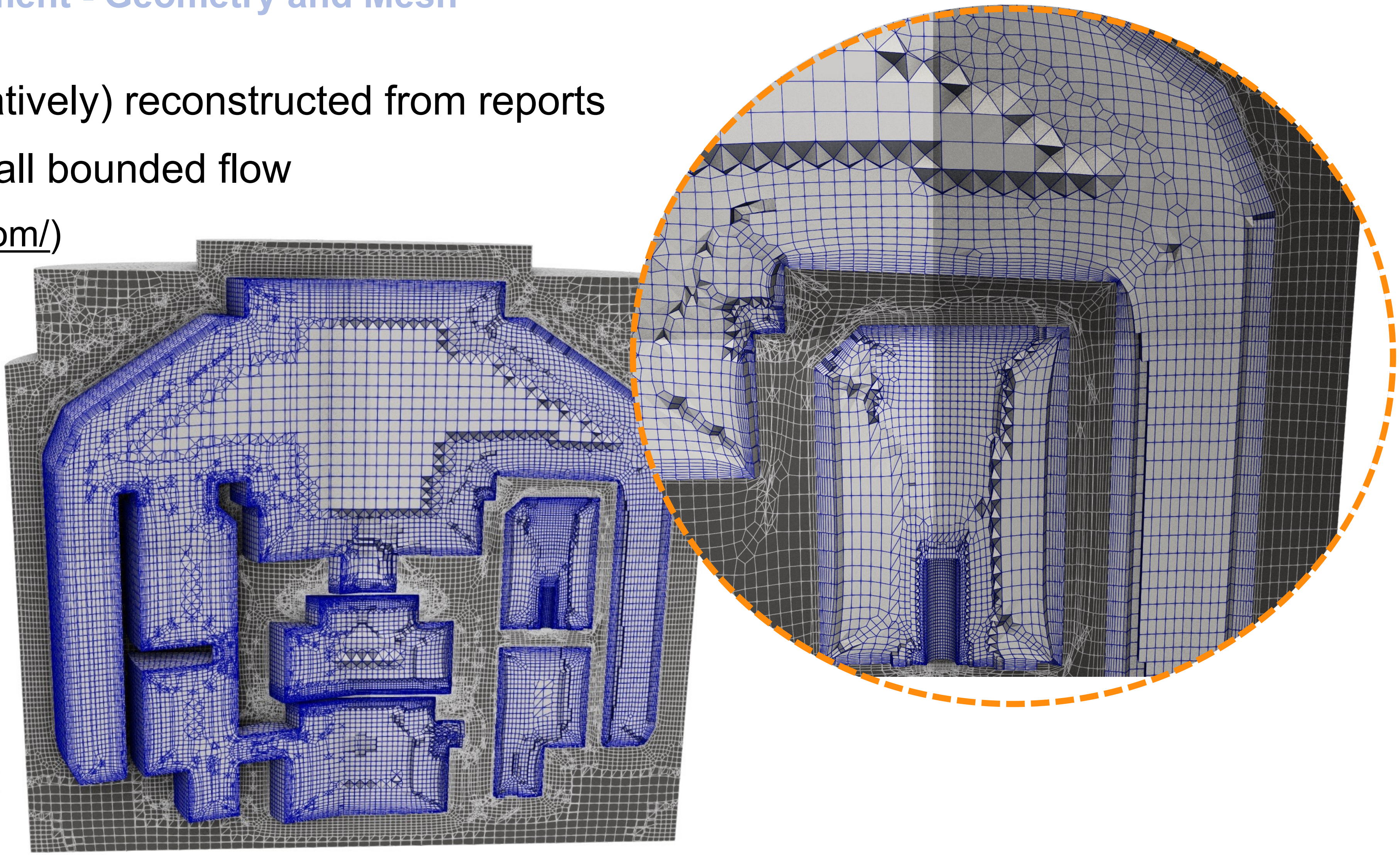
APPLICATION EXAMPLES

ISP37 - VANAM M3 Experiment - Geometry and Mesh

- Geometry (partly qualitatively) reconstructed from reports
- Multi-compartmented wall bounded flow
  - CF-MESH+ (https://cfmesh.com/)

Mesh statistics:

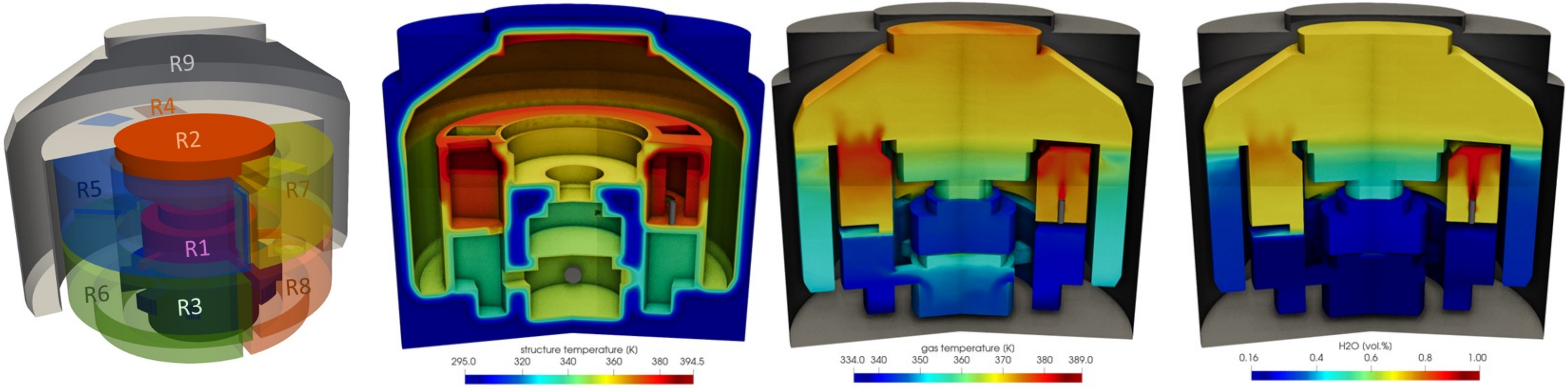
- Solid cells: 1.97 mill
- Fluid cells: 2.55 mill
- min. face angle > 10°
- ave. face angle ~78°



APPLICATION EXAMPLES

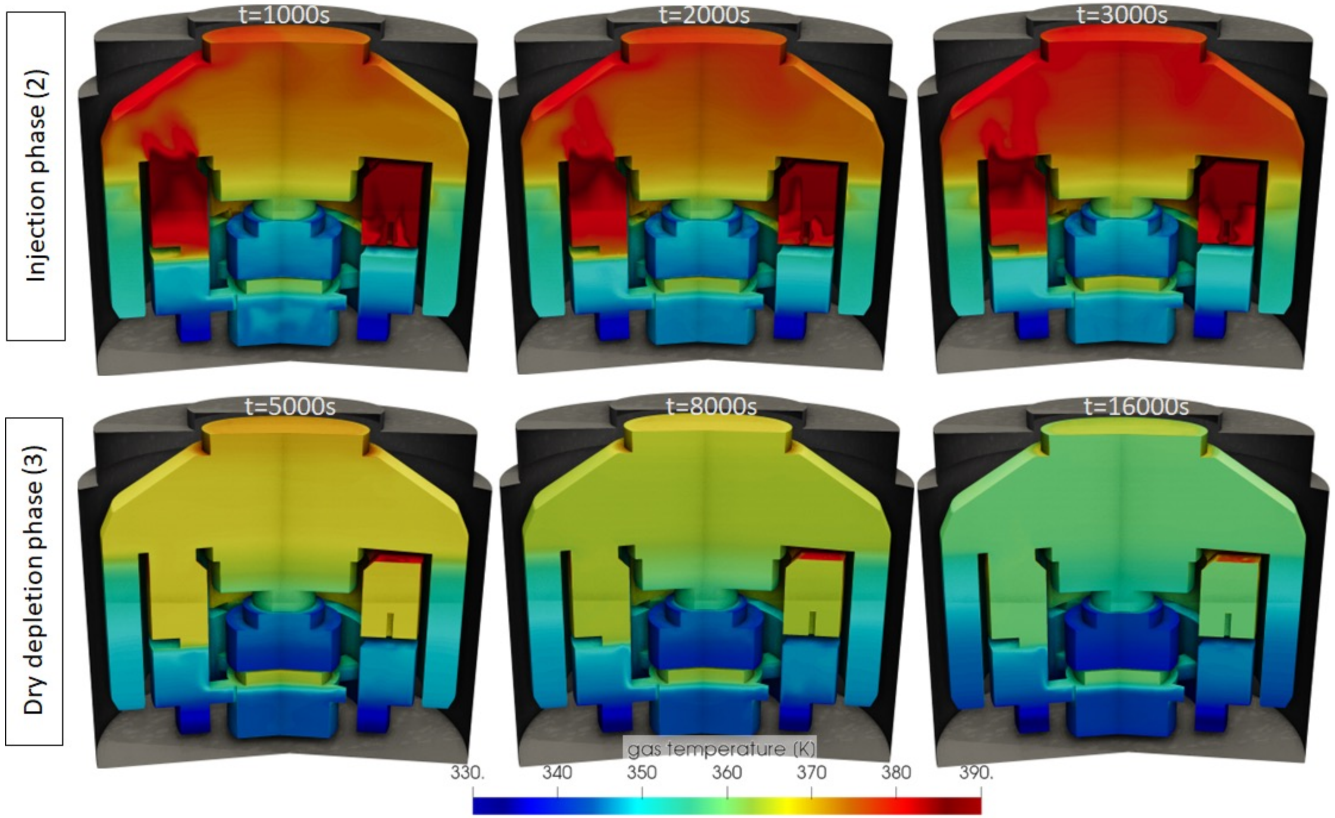
ISP37 - VANAM M3 Experiment - Initial and Boundary Conditions

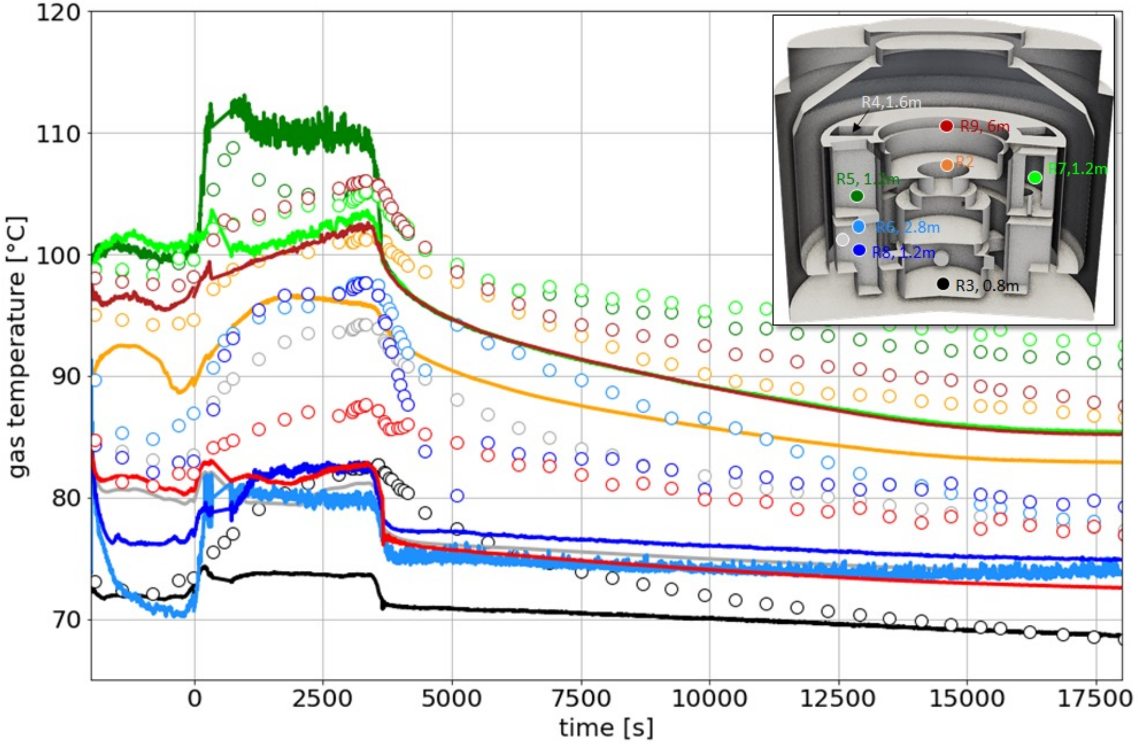
- Avoiding simulating the pre-conditioning phase (~17h) by estimating initial fields:
  - Structures: imposing measured temperatures and diffusing heat for 10.000 s
  - Atmosphere: imposing measured temperatures and run 2.000 s of the transient to obtain 3D turbulent flow field



APPLICATION EXAMPLES

ISP37 - VANAM M3 Experiment - Gas temperature field

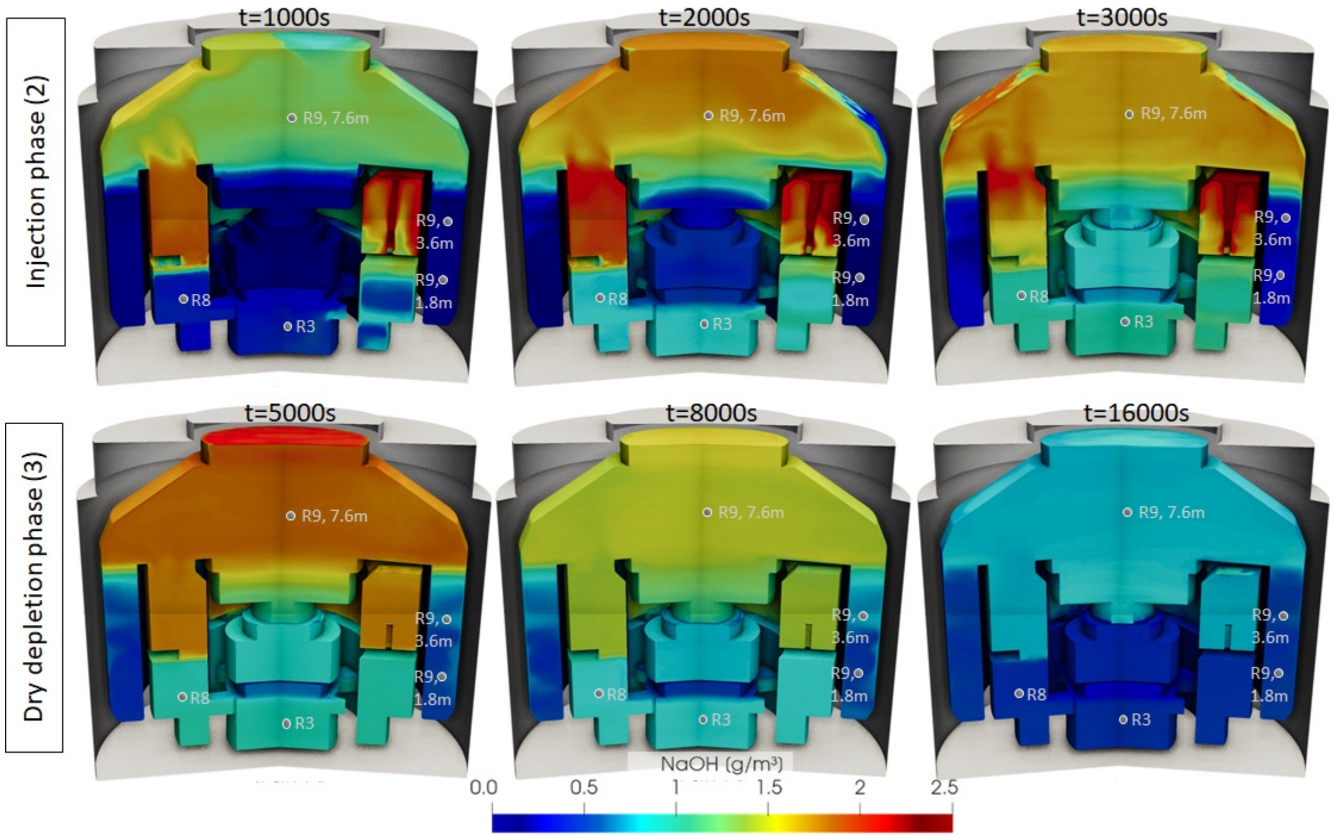


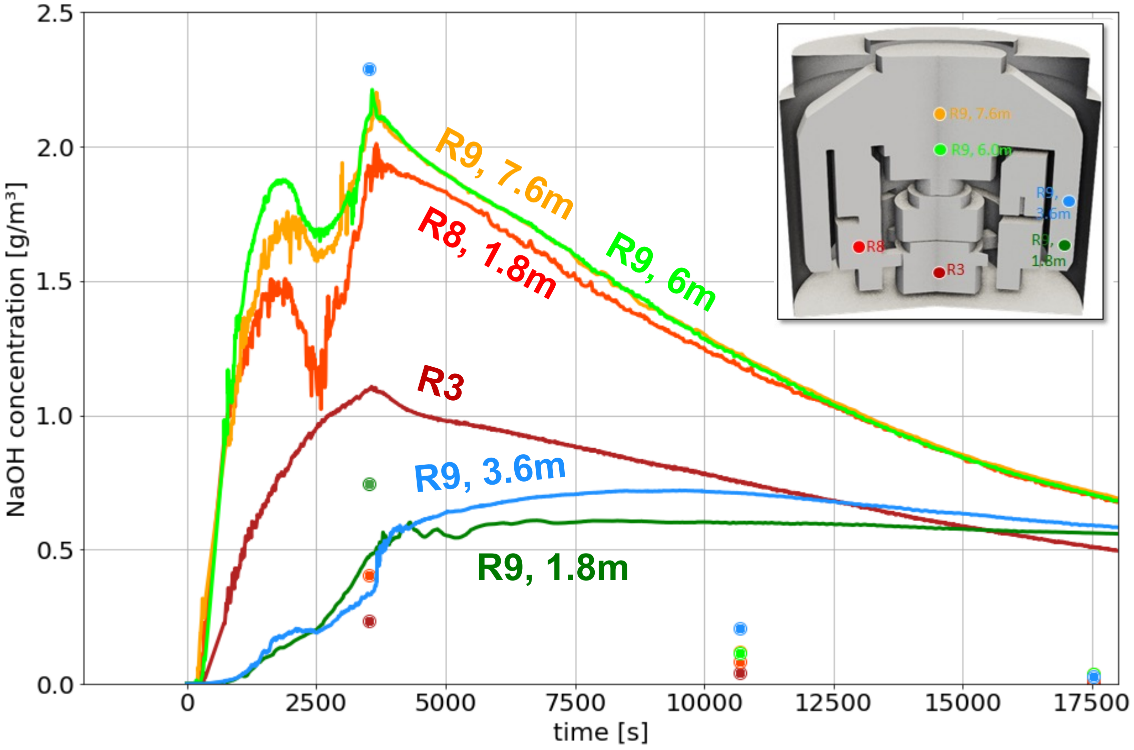


➤ Reasonable predictions above injection (R2, R5, R6, R9) but visible differences below (R3, R8, R4)

APPLICATION EXAMPLES

ISP37 - VANAM M3 Experiment - NaOH aerosol distribution





- Distribution according to flow, however depletion is underpredicted
- Large uncertainties w.r.t size distribution at injection and measurements (only dry samples)

APPLICATION EXAMPLES

ISP37 - VANAM M3 Experiment - Conclusions

- FOAK application containment ∇FOAM package to application scale and coupled aerosol transport
- Challenging case with considerable uncertainties (digitalization, leakage), but
- Plausibility and applicability successfully demonstrated.
- Simulation performance:
  - excellent solver stability
  - 128 Intel Xeon Gold CPU @ 3.80 GHz, 4x96 GB RAM, Infiniband network (~20 k cells/core)
  - transient time: 400-700 s/d depending on phase ($\Delta t < 0.03s$; $CFL<10$)
  - significant impact of injection modeling / resolution (here w_{inlet} ~15 m/s) → explore simplifications

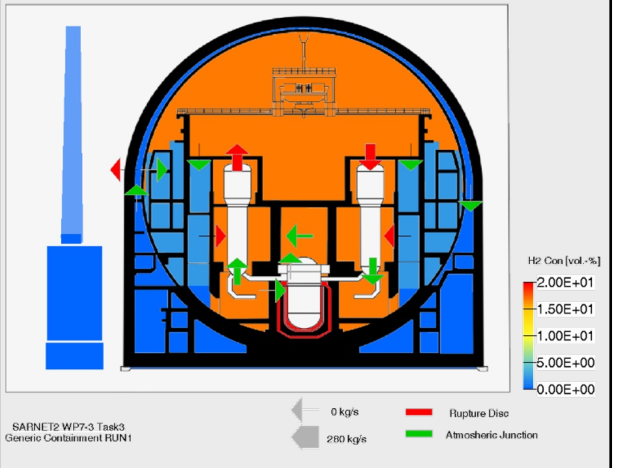
➢ Methodology is ‘application ready’ but still expensive for several hours' long transients

APPLICATION EXAMPLES

EU-AMHYCO 'Towards an Enhanced Accident Management of the H_2/CO combustion risk'

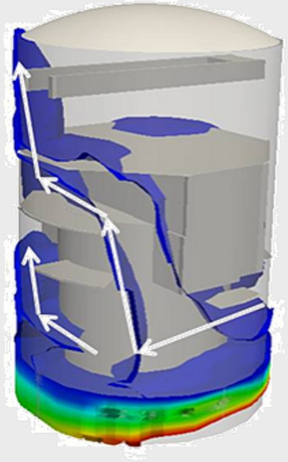
- Work package 4: Full Containment Analysis (01/2023 – 04/2024)
  - Comparative analysis of Containment response conducted for generic KWU, VVER and Westinghouse/French PWR

LP / System codes
(most penalizing scenarios)



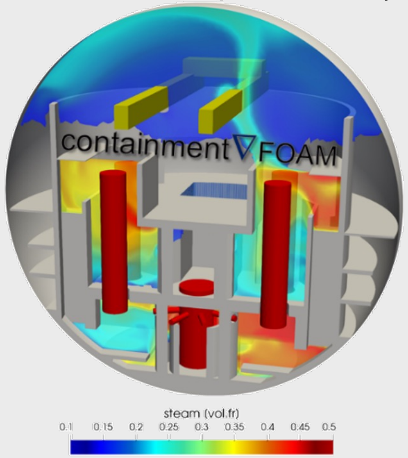
Ref: RUB

GOTHIC-3D
(selected transients)



Ref: UPM

CFD
(selected compartments)



Ref: JÜLICH

- combustion risk
- effectiveness of mitigative measures
- equipment surveillance
- instrumentation representativeness

➢ Provide basis for revision of late phase SAMG (WP5)

📖 Jimenez, G., et al.. AMHYCO Project – Towards and Enhanced Accident Management of the H2/CO Combustion Risk, NURETH-19, 2022.

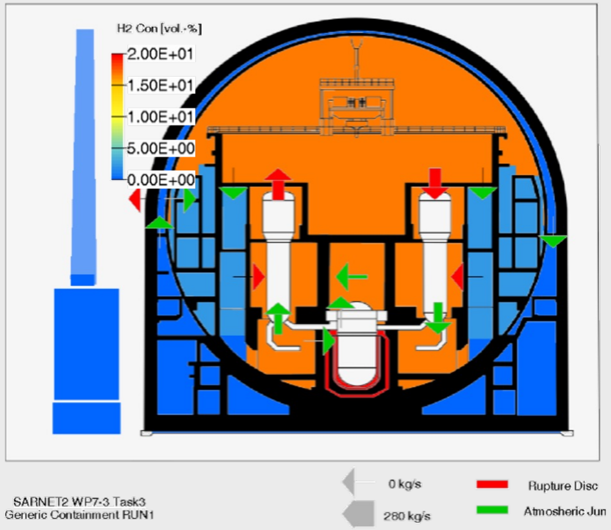
APPLICATION EXAMPLES

Integration in the Analysis Chain – Assessment of Combustion Loads

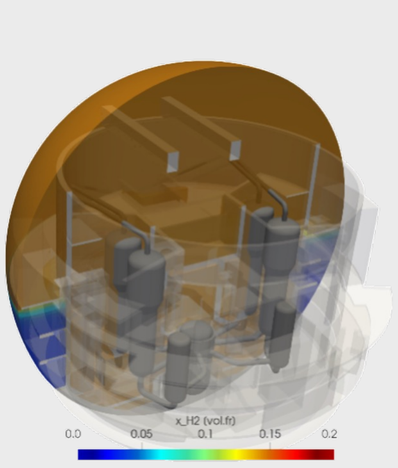
Supported by: Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection

based on a decision of the German Bundestag Fkz 150 1573

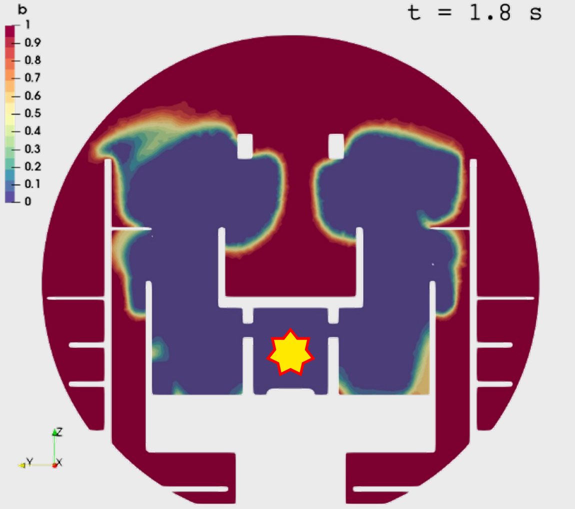
- Initialization of CFD combustion load analysis from system codes (Hasslberger et al., NED 320, 2017)



system code:
gas composition, T, p per CV

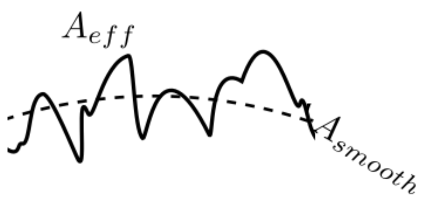


mapping to 3D mesh and diffusing fields



combustion solver
'explosionDynamicsFoam' [1],

Flame wrinkling factor



$$\Xi = \frac{S_{eff}}{S_L} \approx \frac{A_{eff}}{A_{smooth}}$$

Flame wrinkling due to **turbulence** or flame **instabilities** enhances the combustion rate.

➢ Challenge: flame propagation characteristics depend on flow field and turbulence level, which cannot be obtained from system codes!

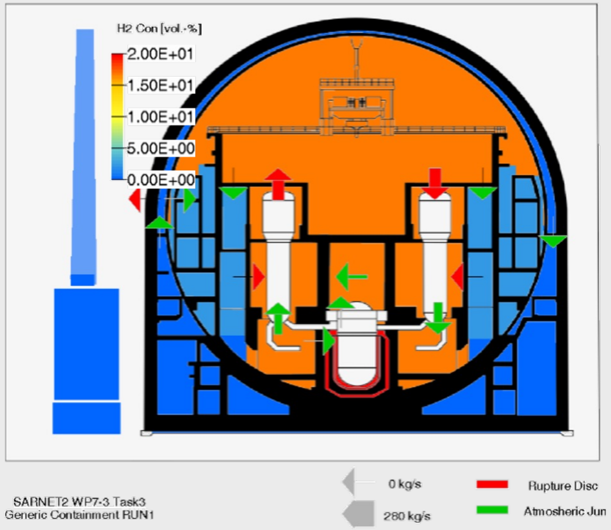
credits to D. Zivkovich

Zivkovic, D., Sattelmayer, T. Towards efficient and time-accurate simulations of early stages of industrial scale explosions. Proc. ICHS 2021.

APPLICATION EXAMPLES

Integration in the Analysis Chain – Assessment of Combustion Loads

- Initialization of CFD combustion load analysis from system codes (📖 Hasslberger et al., NED 320, 2017)



system code:
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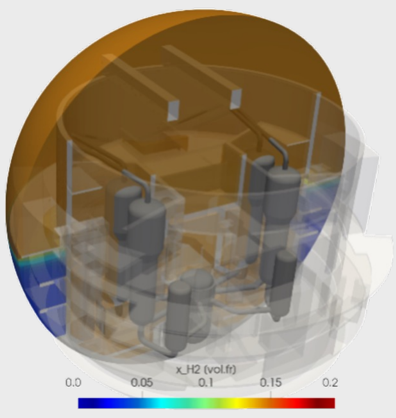
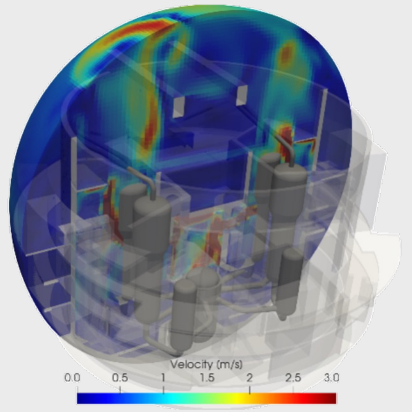
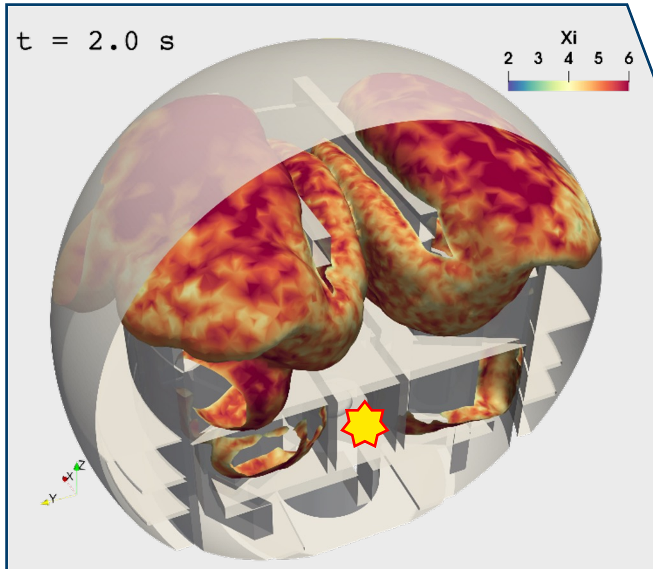


mapping to 3D mesh



containmentFOAM
compute 3D flow field



combustion solver
'explosionDynamicsFoam'

➢ Solution: 3D buoyancy driven turbulent flow field is estimated as IC by running a short transient (here t=360s) before mapping to the combustion solver

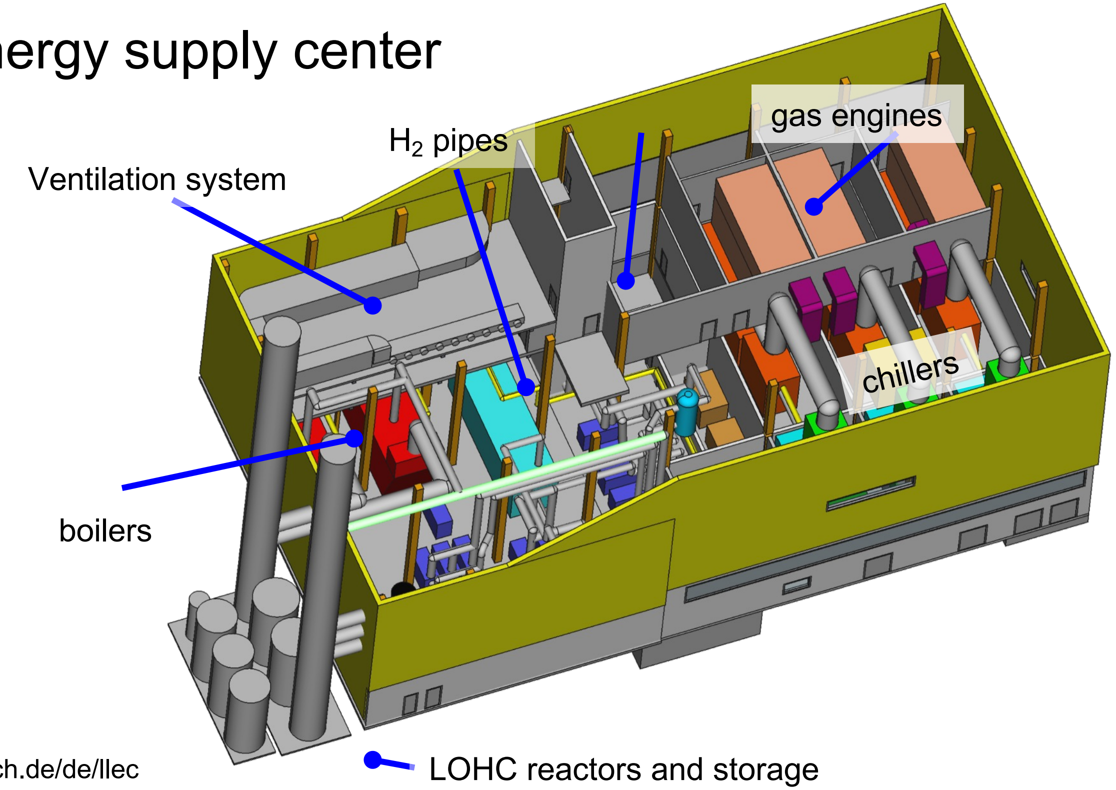
credits to D. Zivkovich

📖 Zivkovic, D., Sattelmayer, T., 2022. Fractal Based, Scale-adaptive Closure Model for Darrieus--Landau Instability Effects on Large-scale Hydrogen-air Flames. Combustion Science and Technology (Accepted).

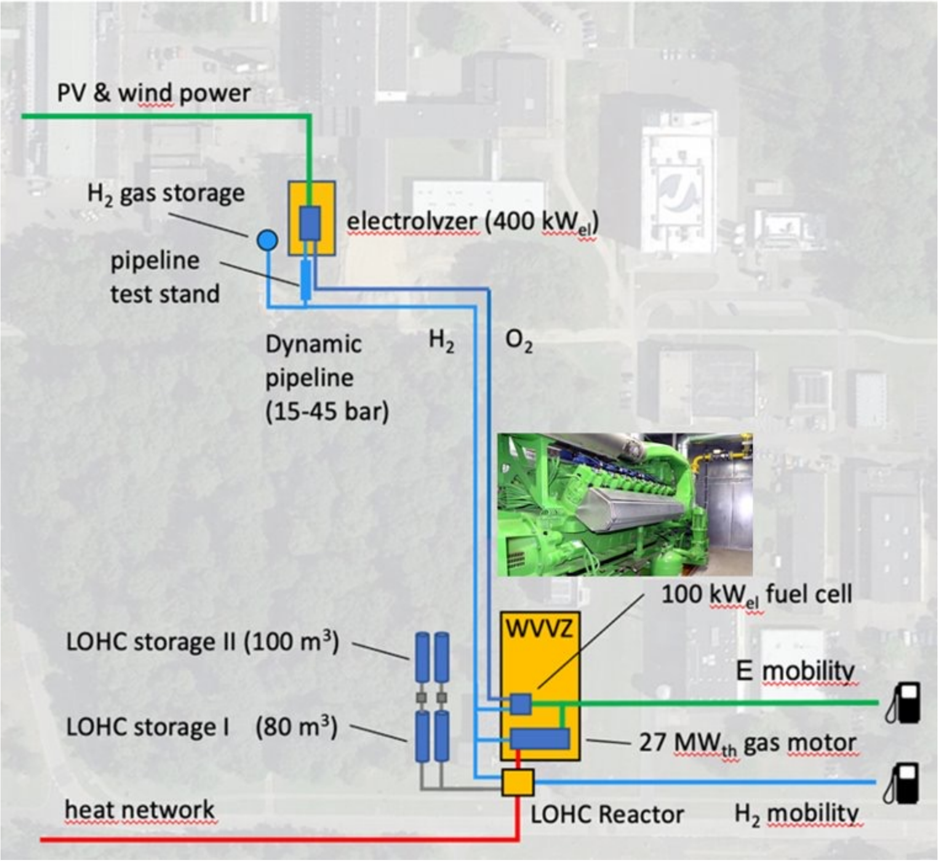
APPLICATION EXAMPLES

Living Lab Energy Campus (LLEC)

- Scientific technological platform for the development of highly integrated energy systems and predictive control strategies for heat, electricity, storage and mobility
- Central energy supply center



https://www.fz-juelich.de/de/llec

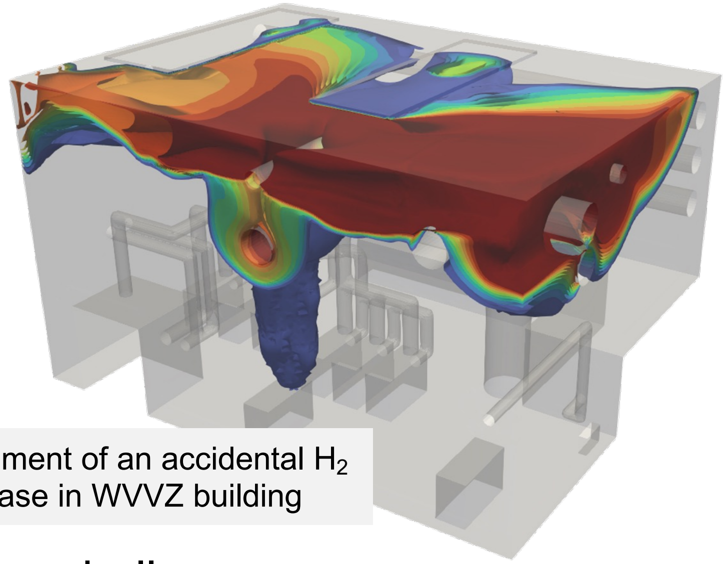


credits to K. Yassin

APPLICATION EXAMPLES

Living Lab Energy Campus (LLEC)

- Pre-normative safety research supporting R&D and future technical applications of sector-coupled energy systems



Assessment of an accidental H_2 release in WVVZ building

Standards & Safety Principles EHSS, HySAFE, ICHS

3D CFD containment∇FOAM

- Modeling challenges:
  - Model D&V for different (environmental) boundary conditions
  - Integration of technical system behavior

Hazard identification and assessment

Safety concept

Definition
- Requirements
- Conceptual design

Evaluation
- Sensor distribution
- Availability
- Effectivity of measures

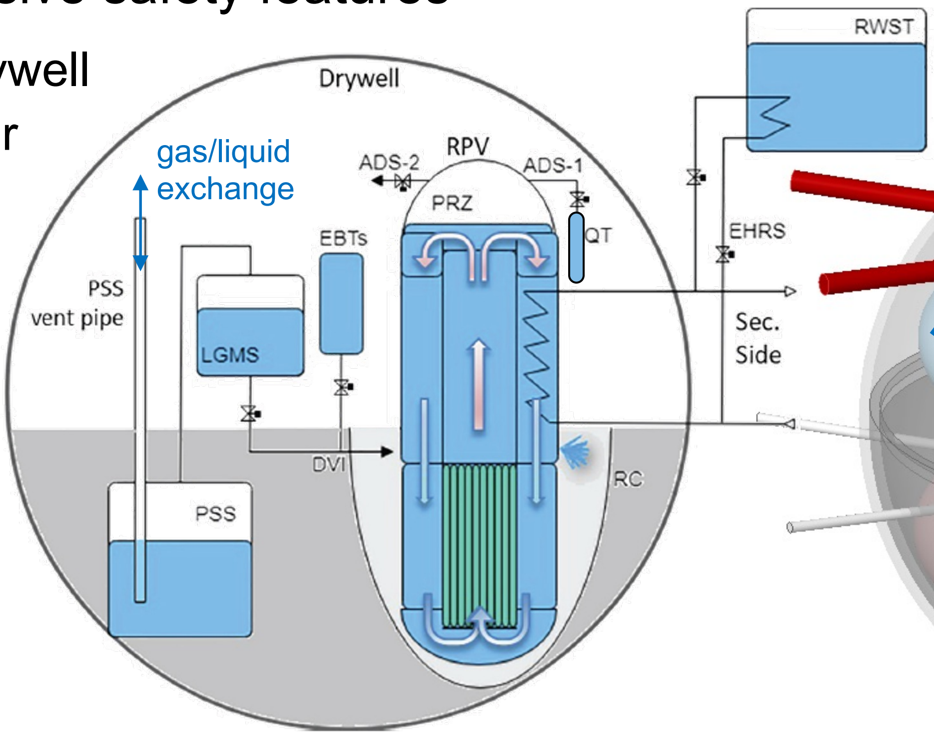
Prevention of flammable H_2-air mixtures

credits to K. Yassin

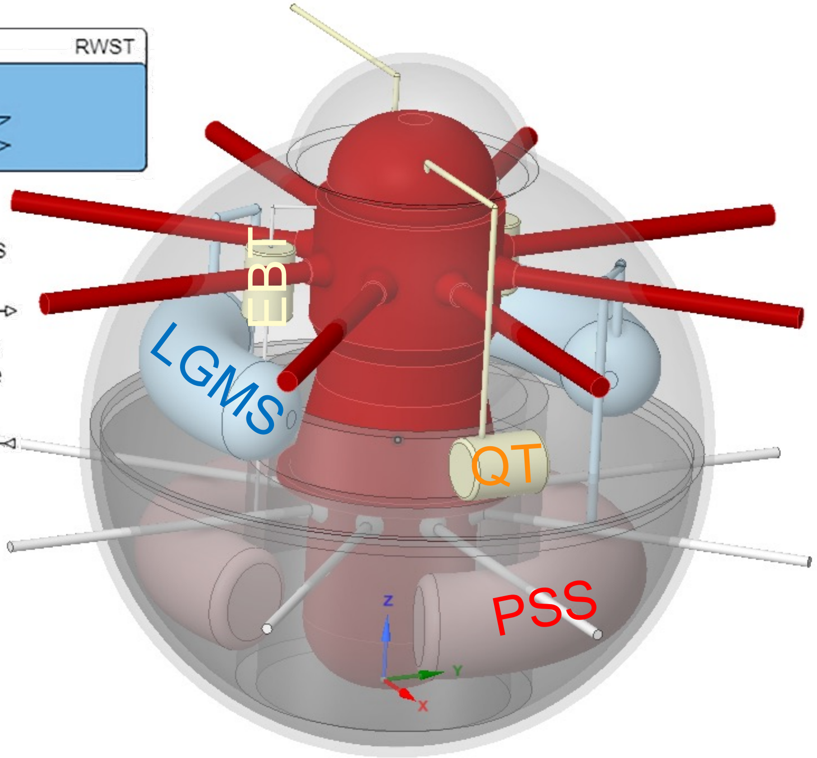
APPLICATION PERSPECTIVES

SMR Applications

- Example: iPWR concept with passive safety features
  - Containment design: N_2 inerted Drywell V~4000m³, PSS V~1000m³, P<9bar
  - DBA pressure up to 9 bar
  - Modeling challenges:
    - Wall condensation at higher pressure and low non-condensable fraction
    - Liquid phase becomes significant (~10% of the free gas volume)
    - Strong interaction with connected LGMS and PSS systems: Condensation and amount of non-condensables stored in their gas space



IRIS iPWR safety concept, figure from Maccari, 2023



IRIS iPWR, own figure

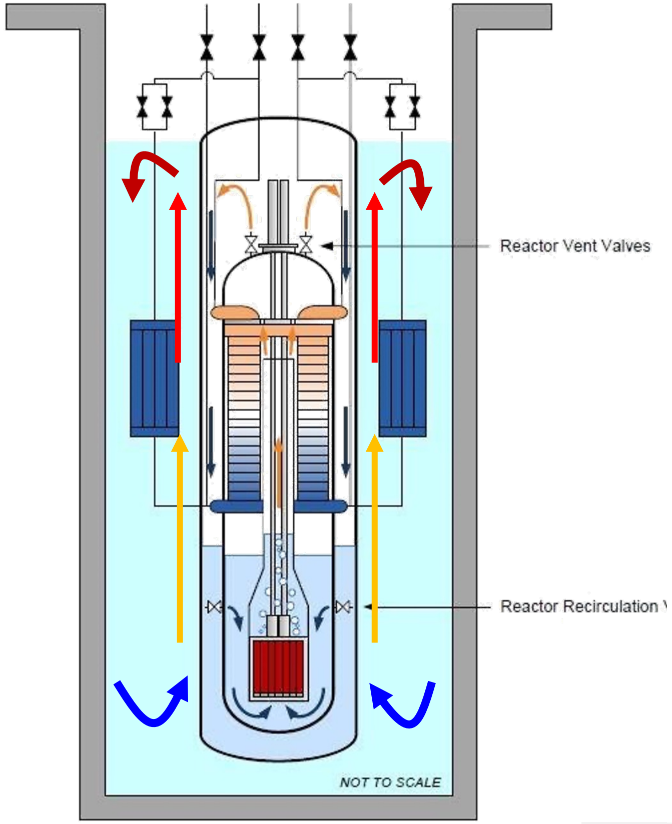
credits to C. Vázquez-Rodríguez

(📖 Di Giuli. Exploratory Studies of Small Modular Reactors Using the ASTEC Code, ICAPP 2015
Maccari et al., Analysis of BDBA sequences in a generic IRIS reactor using ASTEC code, ANE, 2023)

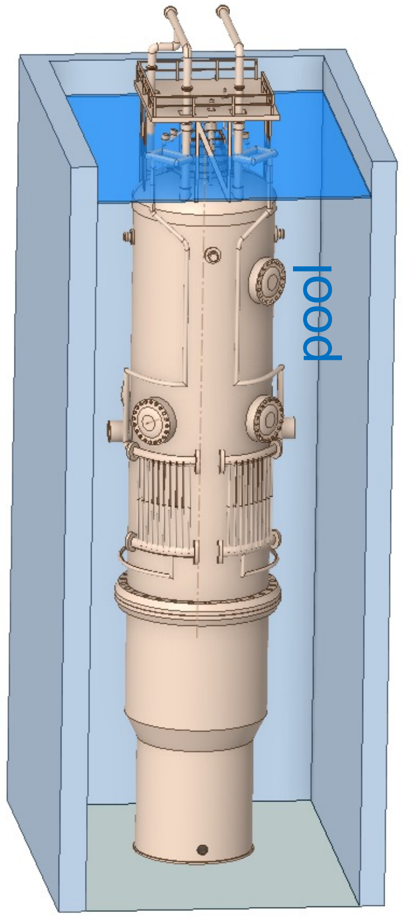
APPLICATION PERSPECTIVES

SMR Applications

- Example: iPWR with submerged containment
  - Containment design: N_2 inerted / evacuated Drywell V~1500-5000 m³, P<50 bar
  - Modeling challenges:
    - Wall condensation at high pressure and low (no) non-condensable fraction
    - Liquid phase becomes significant (considerable part of the free gas volume)
    - Strong interaction with connected external cooling of CV
    - Pool side: High Ra number convective heat transfer (beyond validity of existing emp. Correlations)



NuScale iPWR safety concept, figure from NuScale, 2014



NuScale iPWR, own figure

(📖 Nuscale Power, NuScale Plant Design Overview, 2014 https://www.nrc.gov/docs/ML1432/ML14329B308.pdf

credits to C. Vázquez-Rodríguez

OUTLINE

JÜLICH Forschungszentrum

- Severe Accidents and Containment Analysis
- Development of containment∇FOAM
- Theoretical Background
  - Buoyancy driven turbulent multi-species flows
  - Condensation processes
  - Thermal radiation
  - System models (PARs, code coupling, burst discs, porous models)
- containment∇FOAM framework
  - repository
  - cfGUI and cfSolutionMonitor
- Summary and Conclusions

DEVELOPMENT OF CONTAINMENTFOAM

Strategy and General Considerations

- Coordinated R&D effort (currently 14 active contributors, cumulative > 30 person years R&D)
  - Multi-scale and Multi-physics application:
    - All physical phenomena and their interaction need to be considered to be representative of a accident progression
      - No separate effect consideration possible, models have to be robustly coupled
      - Model basis has to be well balanced in terms of accuracy and efficiency

    - Baseline set of models
      - Model set with known limitations rather than optimal model for a specific condition
      - User guidance for consistent application of the baseline model
      - Limit maintenance effort
  - Framework / quality assurance
    - Guided case setup and solution monitoring
    - Common post processing (functionObjects), data handling and minimum I/O
    - Software framework for uncertainty quantification

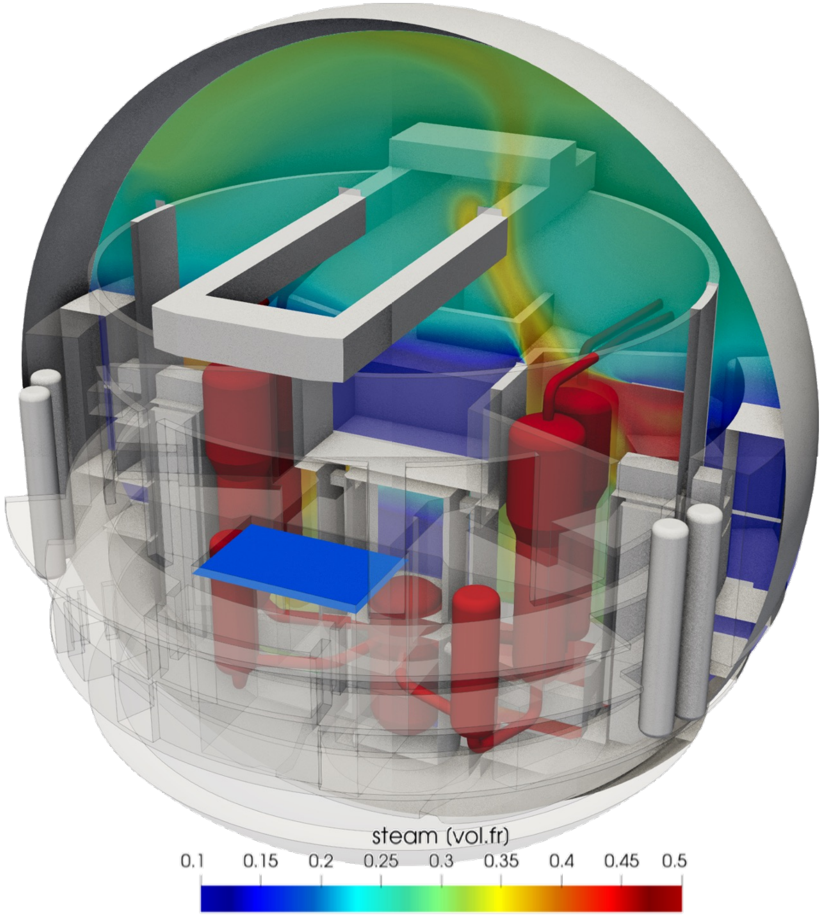
CONTAINMENT ATMOSPHERE MIXING

JÜLICH Forschungszentrum

Pressurization, H2 Risk and Mitigation, Aerosols

- Geometric Complexity
  - Multi-compartmented volume separated by doors or burst discs
  - Wide range of length and time scales
- Phenomenological Complexity
  - Broad range of flow regimes (blow-down to primarily buoyancy driven flows and stagnant zones)
  - Multiple interacting physical phenomena and system feedbacks

➢ A simulation can only be representative if all phenomena and their interactions are considered

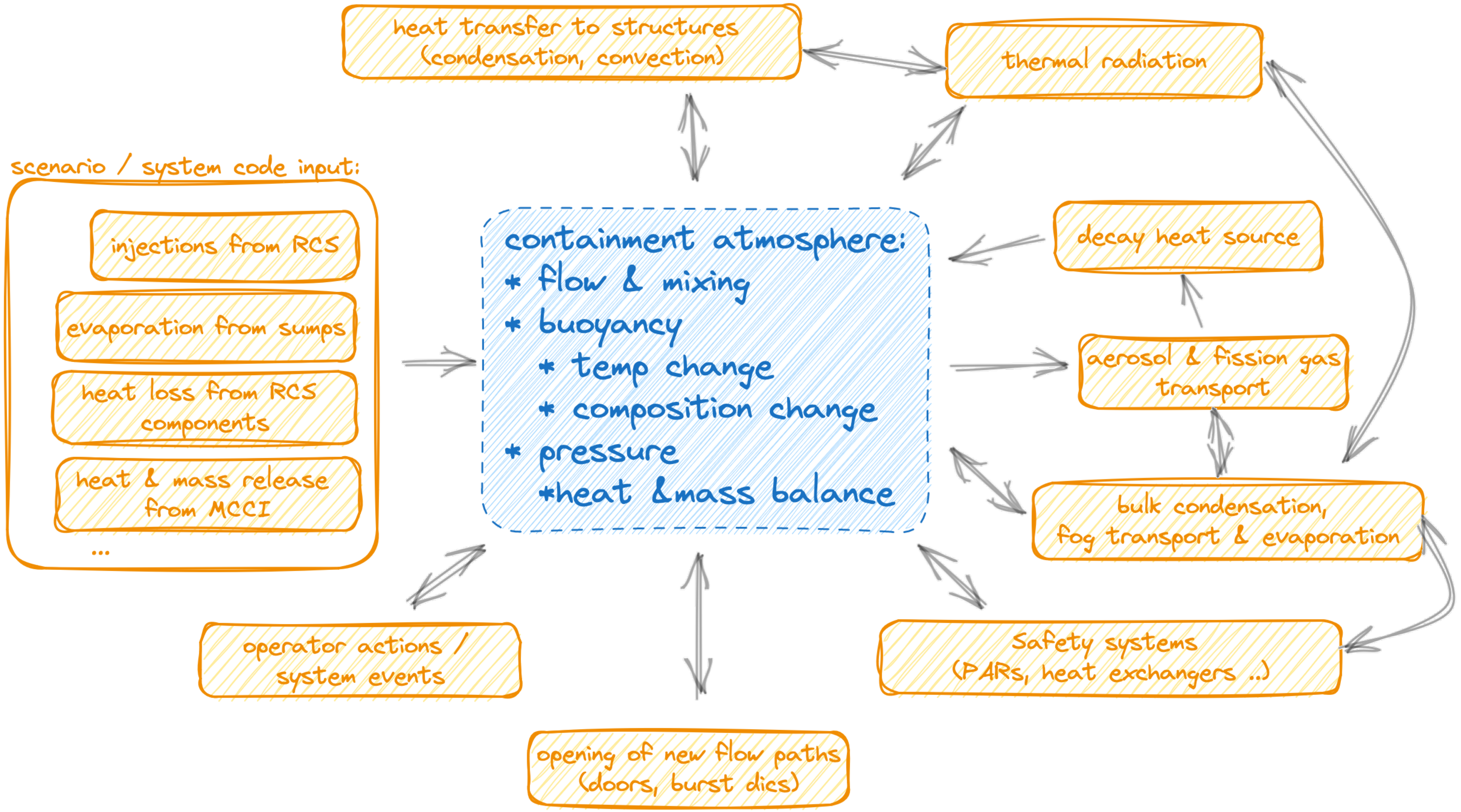


Steam distribution inside a dry PWR containment, 3D CAD Geometry by L. Serra-Lopez (UPM)

R. Liang et al. Status Report on Hydrogen Management and Related Computer Codes, NEA/CSNI/R(2014)8

CONTAINMENT ATMOSPHERE MIXING

Phenomena



CONTAINMENTFOAM AT A GLANCE

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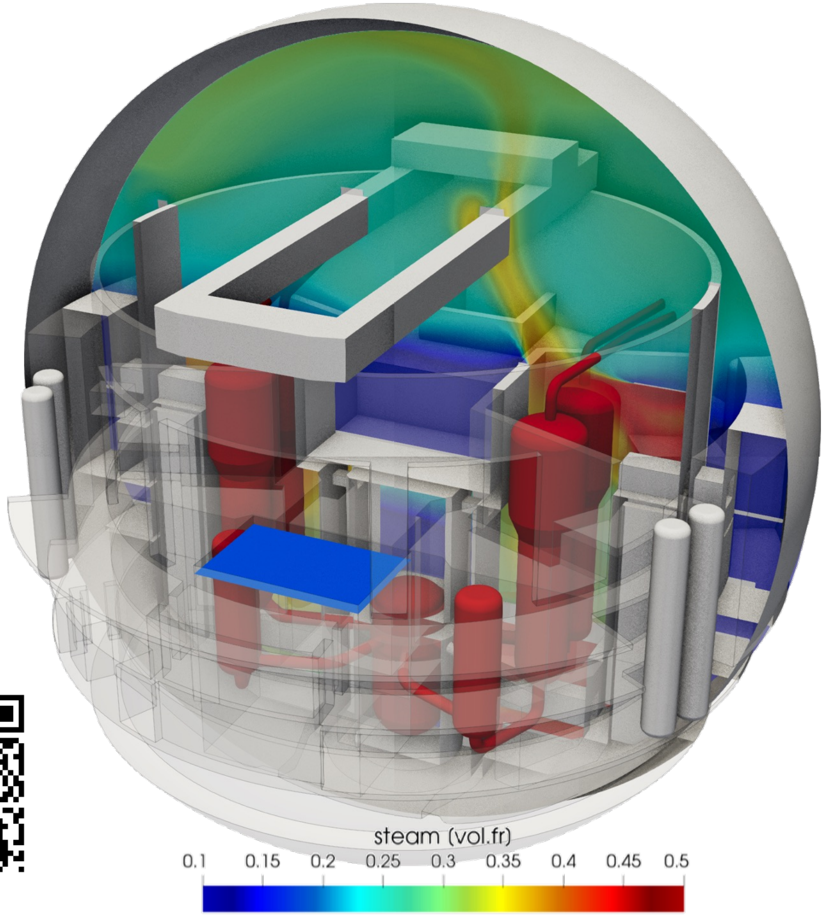
Modeling Pressurization, Aerosol Transport and H_2/CO Gas Mixing and Mitigation

- Flows and Transport Phenomena
  - **Efficient Multi-Species Solver:** effective binary diffusion, Wilke mixture ✓
  - **Turbulence transport**: k-ω SST model with buoyancy terms, ✓
  - **Conjugate heat transfer** ✓
  - **Wall condensation**: single phase diffusion layer model, ✓ implemented as face fluxes, ✓ dedicated wall treatment ✓
  - **Fog formation**: single phase drift flux model ✓ incl. PBM, VOF model ✓
  - **Gas radiation**: Emission-based Reciprocity Monte Carlo Method, ✓ SNBCK and LBL spectral models, ✓
  - **Aerosol transport**: single phase drift flux model, incl. decay heat ✓
- Technical Systems and Components
  - **PARs**: Code coupling with mechanistic model *REKODIREKT* ✓
  - **Burst discs, flaps, doors**: conditional mesh interfaces ✓
  - **Heat exchangers unresolved structures**: porous media ✓
  - **other systems**: Code coupling with OpenModelica ✓



Steam distribution inside a dry PWR containment, 3D CAD Geometry by L. Serra-Lopez (UPM)

Kelm, S. et al. "The Tailored CFD Package 'containmentFOAM' for Analysis of Containment Atmosphere Mixing, H_2/CO Mitigation and Aerosol Transport" *Fluids* (2021) 6, no. 3: 100. https://doi.org/10.3390/fluids6030100

STRUCTURE OF THE CF PACKAGE

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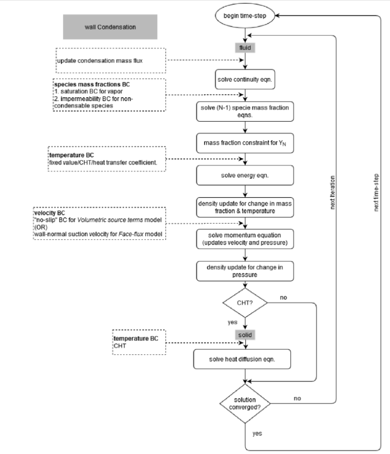
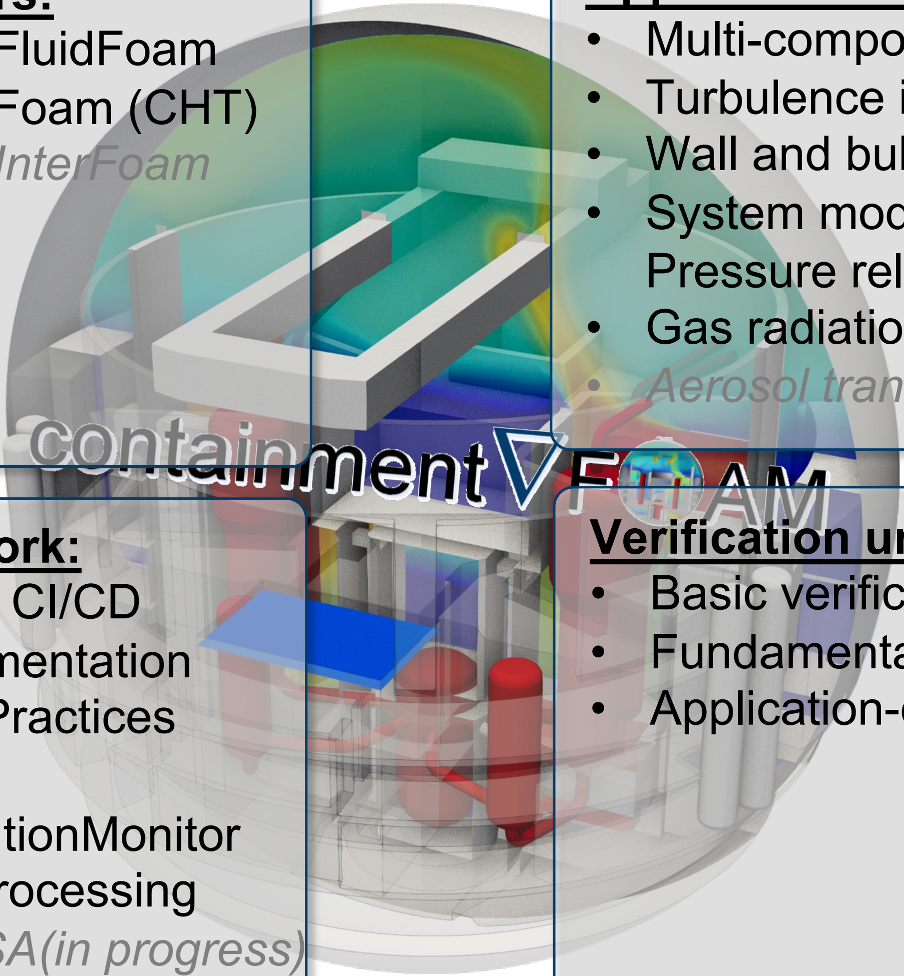


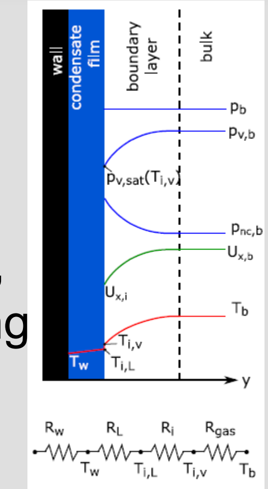
Tailored solvers:

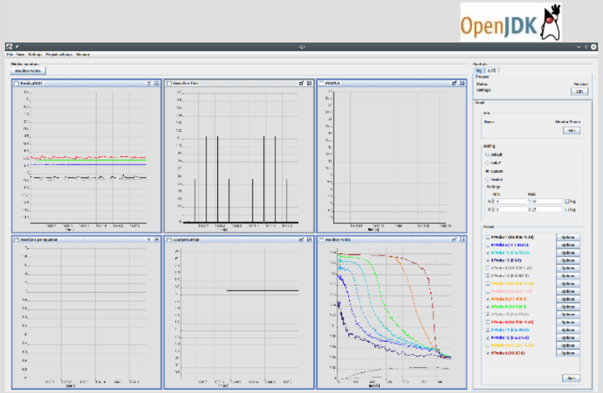
- containmentFluidFoam
- containmentFoam (CHT)
- *containmentInterFoam (in progress)*



Application-oriented Models:

- Multi-component mixtures
- Turbulence in buoyant flows
- Wall and bulk condensation
- System models (H_2-Recombiners, Pressure relief flaps, Heat exchang
- Gas radiation transport
- *Aerosol transport (in progress)*



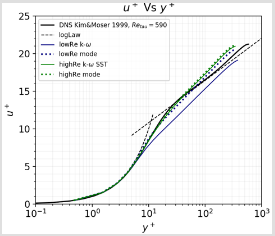


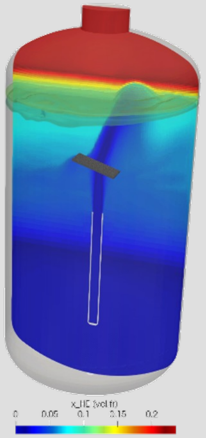
Framework:

- gitlab, CI/CD
- Documentation
- Best Practices
- cfGUI
- cfSolutionMonitor
- postProcessing
- *UQ&SA(in progress)*

Verification und Validation:

- Basic verification
- Fundamental validation
- Application-oriented validation





DESIGN OF CONTAINMENTFOAM

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- Not a stand-alone software, but add-on to OpenFOAM (v9)
- New functionality is added via
  - cloned and modified code (minor extensions)
  - separate base/derived classes (e.g., multispecies, condensation)
    - access information from OpenFOAM
    - conducting plausibility checks during instantiation
    - doing the math
    - provide access functions to solvers/models
    - encapsulated for better maintainability

```
FatalErrorInFunction
<< " Illegal boundary condition for " << U.name() << " field boundary = "
<< mesh.boundaryMesh()[patchi].name()
<< " . Select 'condensingWallVelocity' boundary condition"
<< " .Wall condensation error "
<< exit(FatalError);
```

plausibility check for model use and defined boundary conditions

```
//- Update fog velocity
condensation->bulkUFogCorrect();

//- Compute sum of uFog and uDrift volumetric flux fields
phiFog = fvc::flux(condensation->bulkUFog()) + fvc::flux(condensation->bulkUDrift(g));

fvScalarMatrix fogEqn
(
    fvm::ddt(fog)
  + fvm::div(phiFog, fog, "div(phi,fog)")
  ==
    fvm::laplacian((massDiffusion->Dt(0) + condensation->bulkDBrownian()), fog)
  + condensation->bulkMassTransferRate()
);
```

access functions used in the solver. Here fogEqn.H

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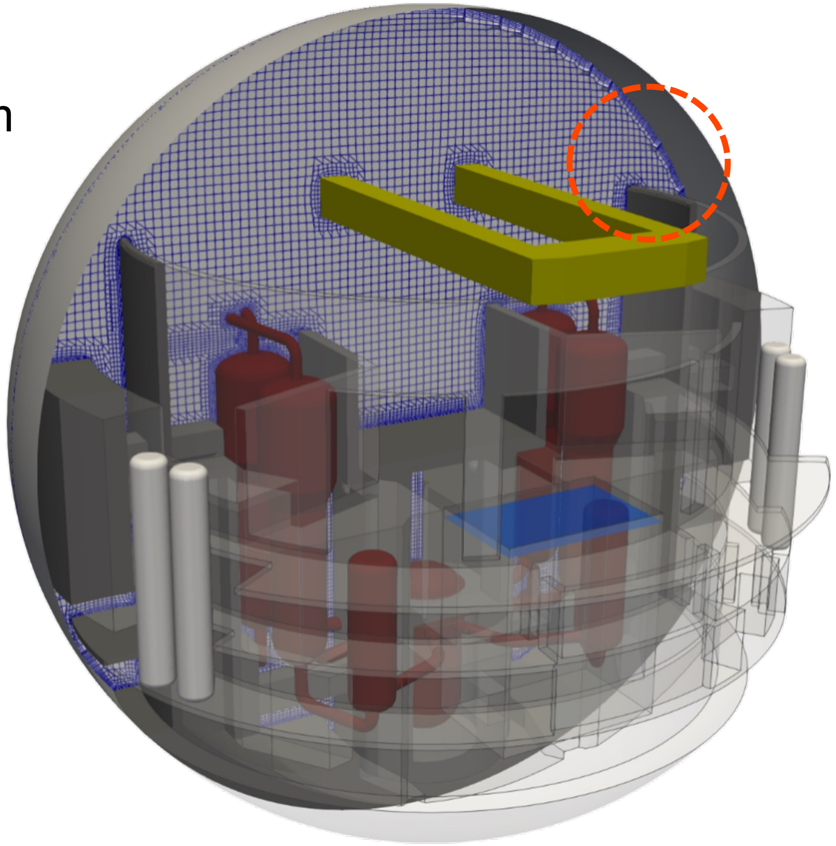
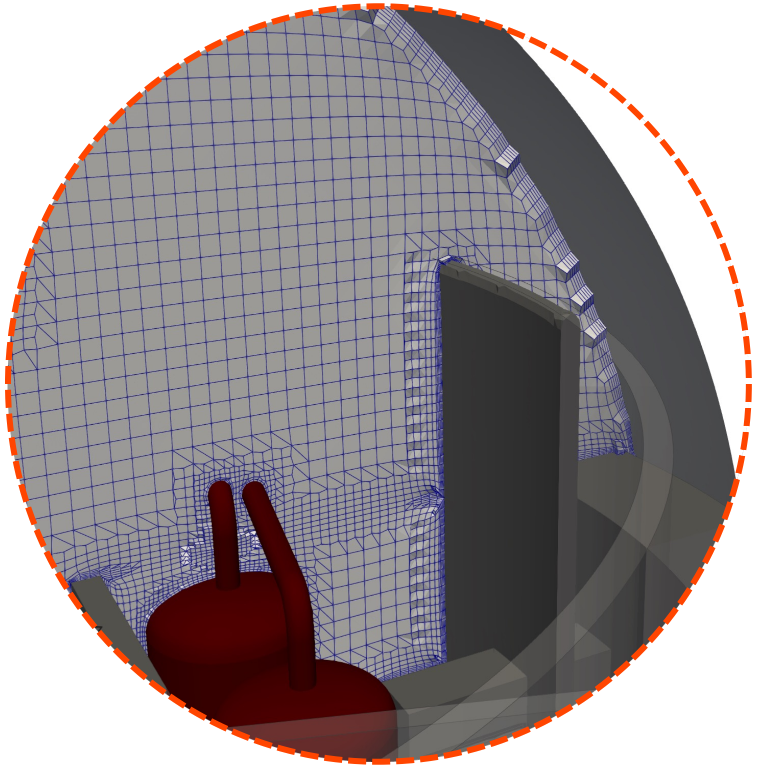
GEOMETRIC MODELING

- Modeling internal flow and transport processes is tightly linked to modeling (simplification) of the complex bounding geometry! → balance the computational effort
  - here, max edge length 0.5m
  - refinement levels 2 → 0.125m
    - ➢ Geometric features of L > 0.25m can be resolved
  - High refinement near structures leads to excessive number of boundary layer cells





CONTAINMENT ATMOSPHERE MIXING

Balanced Modeling

- The solution accuracy is limited by the simplest model, its efficiency by the most expensive model → balanced level of detail required
- Reduction of modeling complexity:
  - Single phase / mixture model
  - uRANS modeling
    - Wall-bounded flow (wall functions)
    - Buoyancy effects
  - Eulerian treatment of fog (& aerosols)
  - Code coupling / porous media
    - PARs, heat exchangers, pressure suppression systems ..
    - System feedback
    - Unresolved structures (walking grids)

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MULTI-SPECIES TRANSPORT SOLVER

Governing Equations (U-RANS form)

- containment∇FOAM
  - Continuity: $$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{U} \right) = \dot{S}'''_m \qquad \rho = \frac{pM}{RT}$$
  - Momentum: $$\frac{\partial \left(\rho \vec{U} \right)}{\partial t} + \nabla \cdot \left(\rho \vec{U} \otimes \vec{U} \right) = -\nabla p + \nabla \cdot \tau + \rho \vec{g} + \dot{S}'''_u \qquad \tau = \rho \left(\nu + \nu_t \right) \left[\nabla \vec{U} + \left(\nabla \vec{U} \right)^T - \tfrac{2}{3} \delta \nabla \cdot \vec{U} \right]$$
  - Species: $$\frac{\partial \left(\rho Y_i \right)}{\partial t} + \nabla \cdot \left(\rho \vec{U} Y_i \right) = \nabla \cdot \left[\rho \left(D_{i,m} + \frac{\nu_t}{Sc_t} \right) \nabla Y_i \right] + \dot{S}'''_y$$
  - (Fluid) Energy: $$\frac{\partial \left(\rho h_{tot} \right)}{\partial t} + \nabla \cdot \left(\rho \vec{U} h_{tot} \right) = \rho \vec{U} \cdot \vec{g} + \frac{\partial p}{\partial t} + \underbrace{\nabla \cdot \left[\rho \left(\lambda + \frac{c_p \nu_t}{\mathrm{Pr}_t} \right) \nabla T \right]}_{\text{conduction}} + \underbrace{\sum_{i=1}^{n} \nabla \cdot \left[\rho h_i \left(\rho D + \frac{\nu_t}{Sc_t} \right) \nabla Y_i \right]}_{\text{multi-component enthalpy diffusion}} + \dot{S}'''_h$$
  - (Solid) Energy: $$\rho \frac{\partial c T_s}{\partial t} = \nabla \cdot \left(\lambda_s \nabla T_s \right)$$

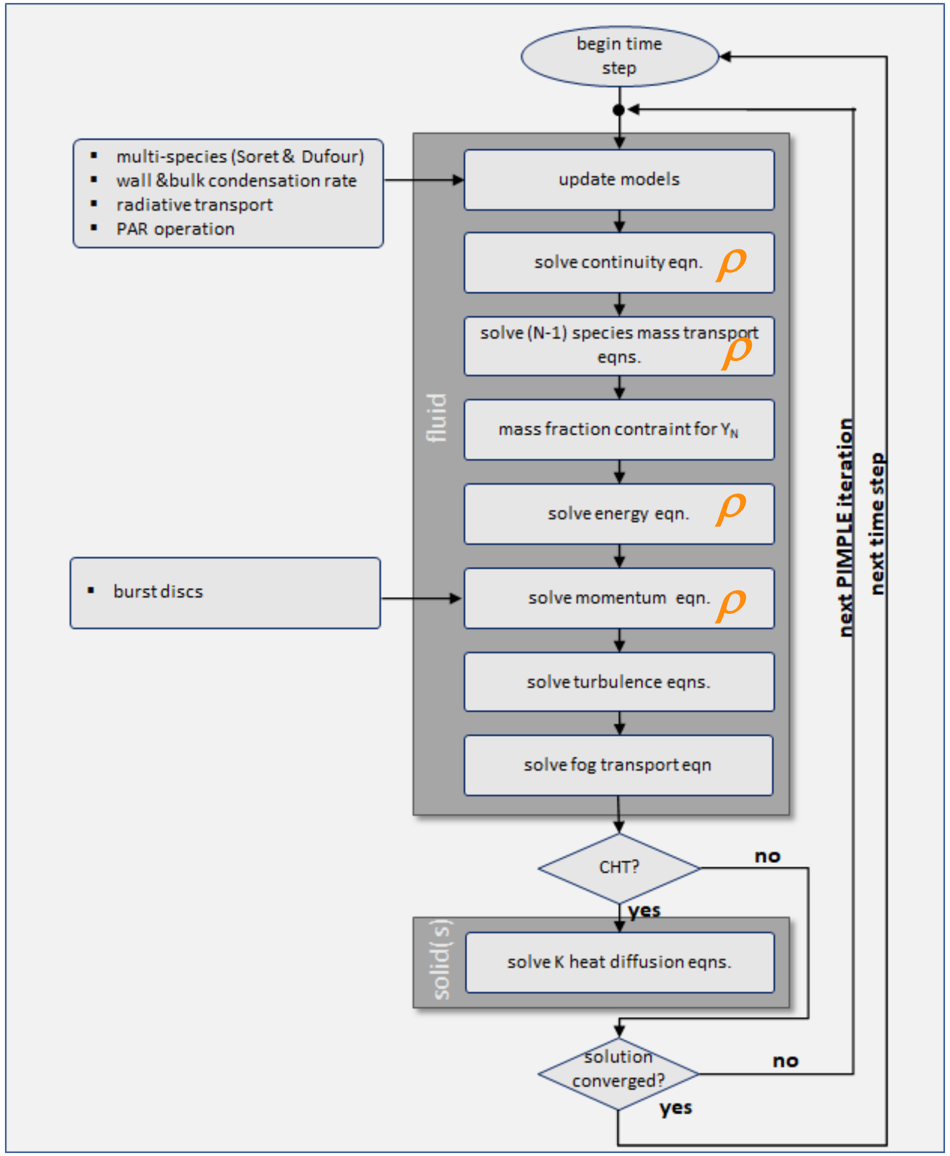
➢ Model implementation via source terms $\dot{S}'''_m, \dot{S}'''_u, \dot{S}'''_y, \dot{S}'''_h$ and boundary conditions

[1] Kelm, S. et al. "The Tailored CFD Package 'containmentFOAM' for Analysis of Containment Atmosphere Mixing, H_2/CO Mitigation and Aerosol Transport" *Fluids* (2021) 6, no. 3: 100. https://doi.org/10.3390/fluids6030100

MULTI-SPECIES TRANSPORT SOLVER

Solver algorithm and integration of models

- We‘re using PIMPLE to converge on density within the time-step (PISO is not possible)
- Models are mostly integrated explicitly i.e., updated within the PIMPLE loop to ease convergence
- Baseline set of numerical settings for validation cases (high quality mesh, low non-orthogonality)



TIME STEP MANAGEMENT

General Concept

- To maintain numerical efficiency and stability of long transient system analysis runs, the time step has to be dynamically adapted due to
  - a to change in the flow pattern (typically indicated by the **CFL number**),
  - the convergence of the simulation (measured by the **number of PIMPLE loops** required for the previous time step) and
  - approaching **system events** (e.g., opening of a burst disc or activation of a safety system) that may lead to sudden changes of the flow → give control to the models.
- To prevent a crash of the simulation or accumulation of errors, a simulated **time step** should be **repeated** with a reduced time step size if convergence is not achieved within a PIMPLE loop.

D. Schumacher, *„Dynamische Zeitschrittanpassung OpenFOAM basierter CFD-Simulationen “, Bachelor Thesis, FH Aachen. Sept. 2021*

TIME STEP MANAGEMENT

General Concept

- New methods:
  - `hierarchical`: controls first CFL and then number of PIMPLE loops
  - `weighted`: combines both criteria based on weight
- Further controls:
  - `delayAdaptionUntil`: prevent time step reduction due to initialization / convergence issues
  - `repeatTimeStepIf`: enables repetition of timestep with reduced time step size ($\Delta t/2$)

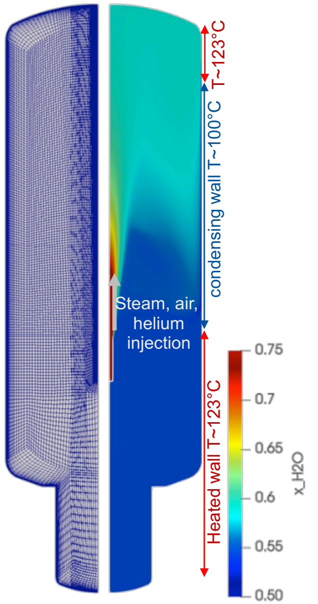
system/controlDict

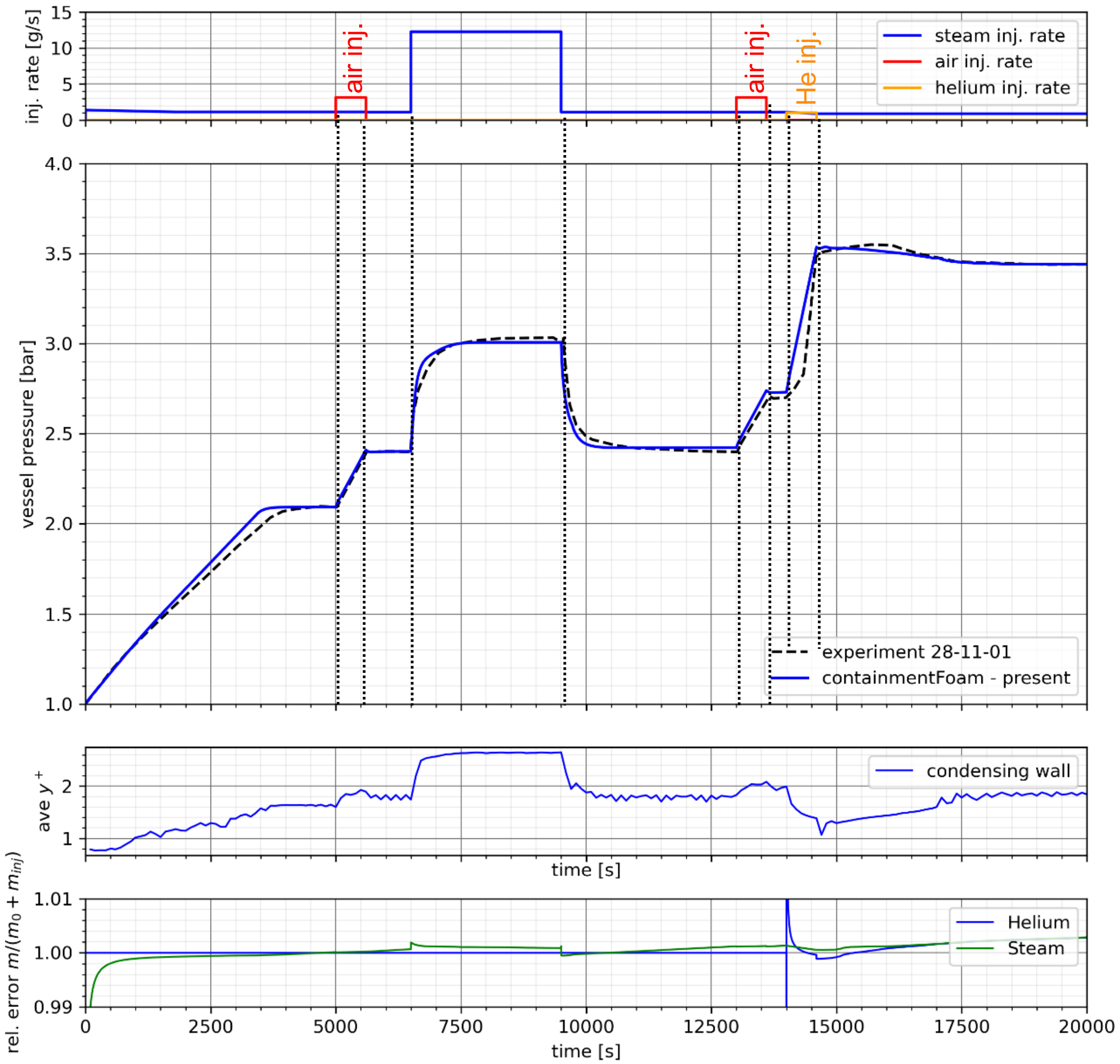
```
adjustTimeStep      true;

timeStepMethod      hierarchical; // hierarchical, weighted, openFOAM, none

delayAdaptionUntil  0.5;      // ignore initial numerical inaccuracy

maxDeltaT           1.0;

timeStepParameter
{
  CourantNumber
  {
    weight            0.6;  // in case of timeStepMethod weighted
    targetValue       5.0;
    repeatTimeStepIf  100;  // set large value to avoid time step repetition
  }

  PIMPLE
  {
    weight            0.4;  // in case of timeStepMethod weighted
    targetValue       10;
    repeatTimeStepIf  21;   // set large value to avoid time step repetition
  }
}
```

TIME STEP MANAGEMENT

Test TOSQAN ISP47

- ISP-47 on containment thermal hydraulics
  - standard regression test for containmentFOAM
  - TOSQAN (7m³) tests
    - 🕮 Malet et al. Nuclear Engineering and Design 240 (2010) 3209–3220
  - Pressurization sequence
  - Verification: mass balance
  - Validation: vessel pressure





TOSQAN-ISP 47 scenario (l) and pressurization transient (r),

TIME STEP MANAGEMENT

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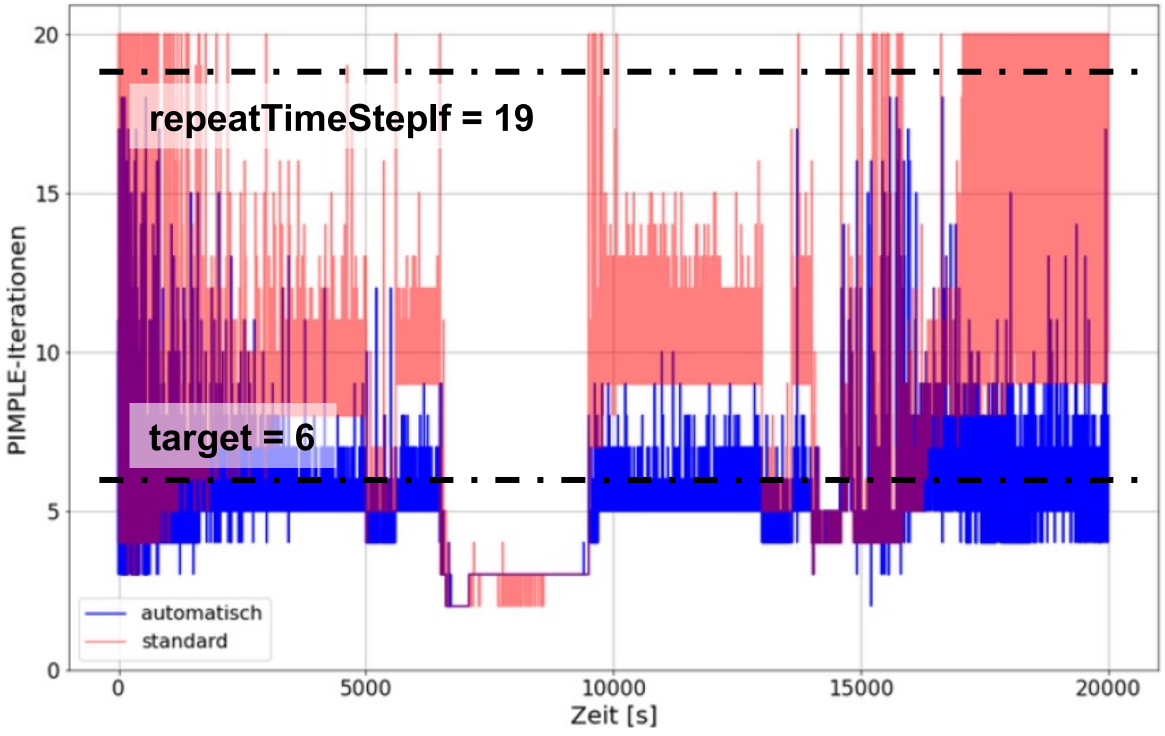
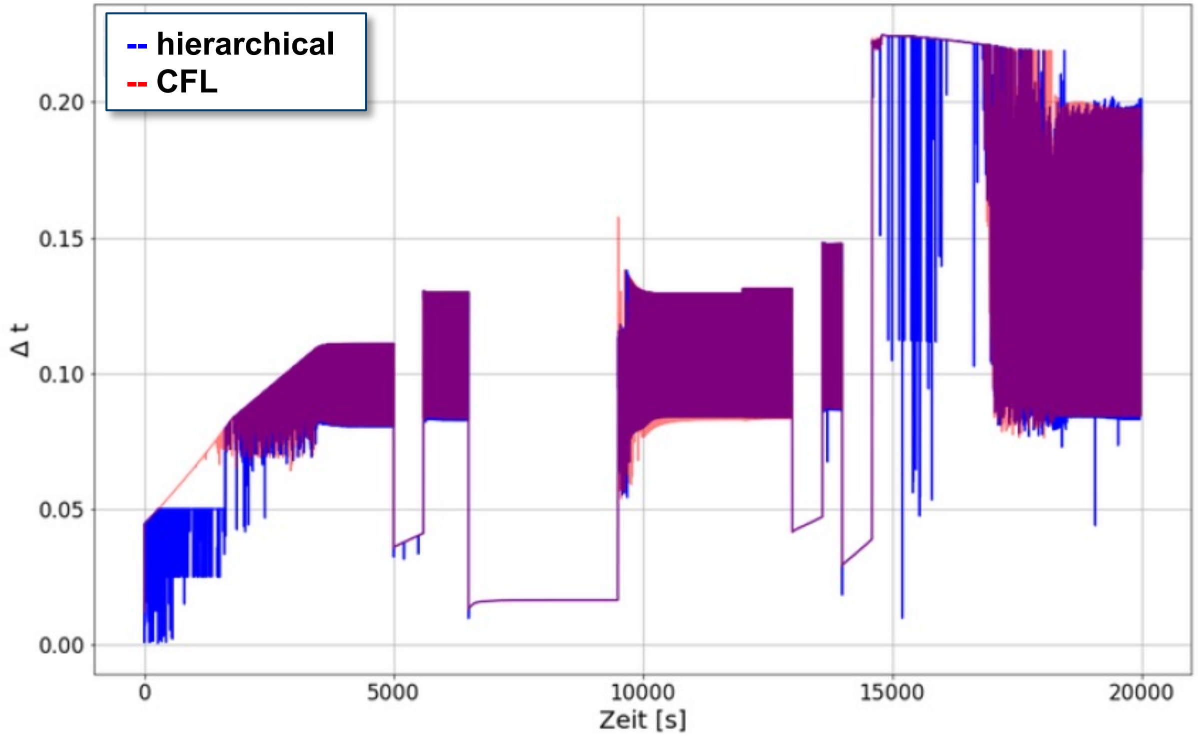
Test TOSQAN ISP47

- Comparison of dynamic time step adaption and convergence





➢ Increased number of time steps from ~370.000 to 380.000

➢ convergence checks (PIMPLE + repetition) lead to visibly less PIMPLE iterations → run time decreased from 37h to 34h

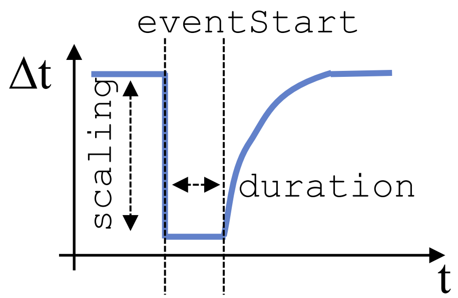
TIME STEP MANAGEMENT

System events (e.g., burst discs)

- Sudden events like a burst disc opening may challenge solver convergence and stability
- Approach: user and models can define system events that reduce the time step before their occurrence
- Controls:
  - `editable`: allows models to change entries
  - `eventStart` : expected occurrence (user defined or calculated in models)
  - `duration`: period for reducing time step before adaptive time stepping takes over control
  - `scaling`: reduction of time step ($\Delta t_{new} = \Delta t/scaling$)

system/systemEvents

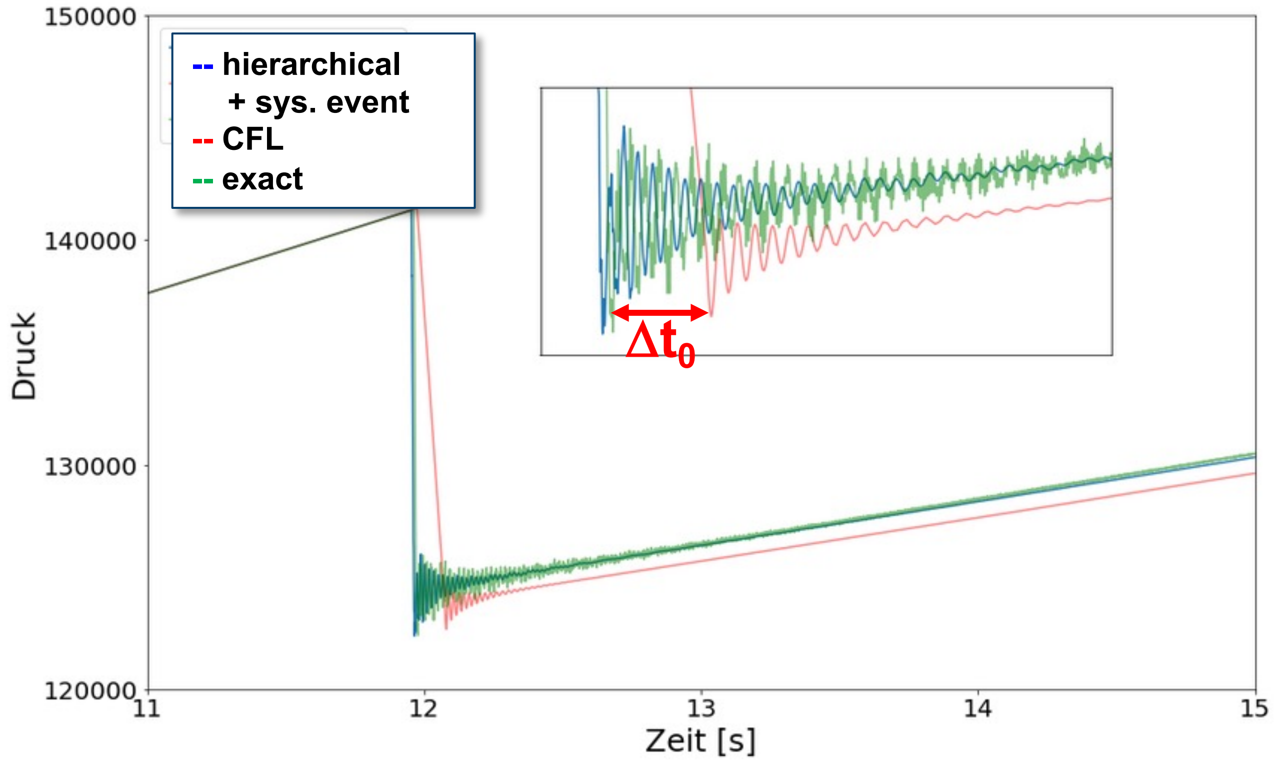
```
events
{
  ExampleEventName
  {
    editable                       true;
    eventStart                     123.5;
    duration                       0.1;
    scaling                        100.0;
  }
}
```

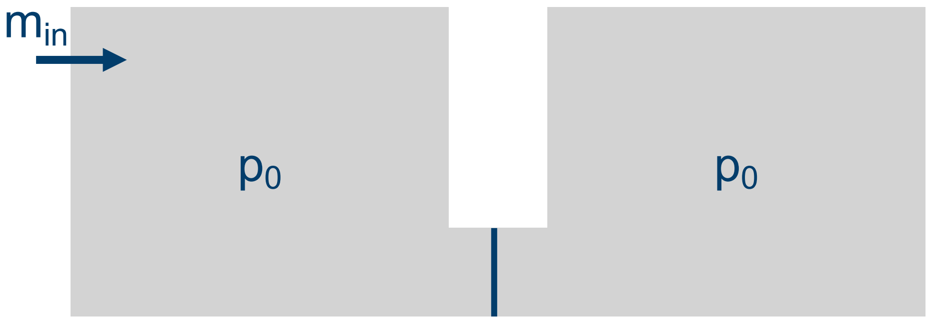


TIME STEP MANAGEMENT

Test burst disc

- Opening of a burst disc:



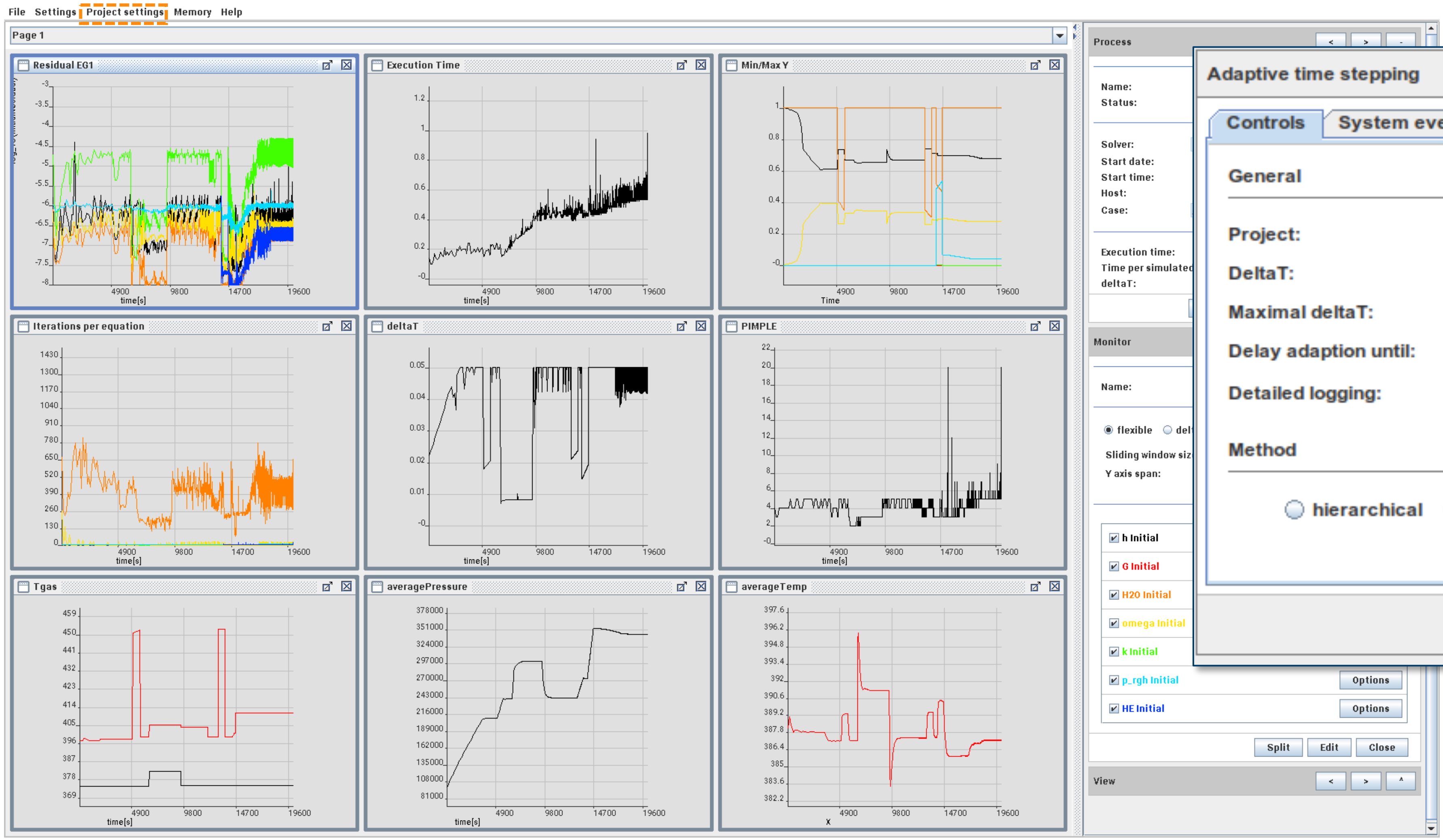


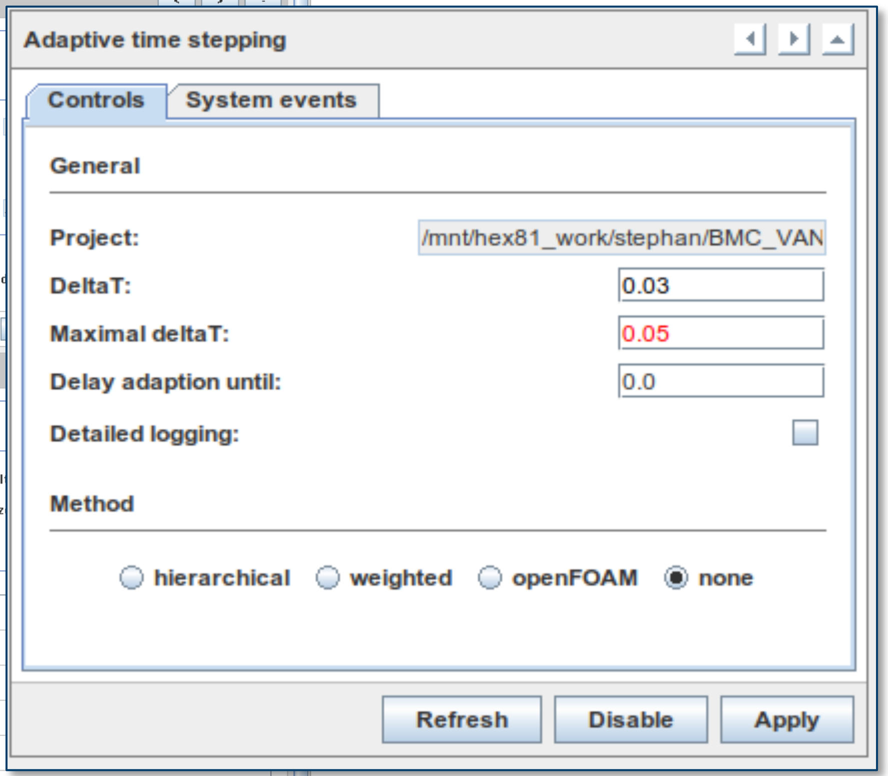
Burst disc test case (r) and pressure history for different time stepping strategies (l)

- ➢ Improved stability, max. CFL < 4 rather than 450, but increased computation time (14 min -> 23 min)
- ➢ Visibly better time resolution and accuracy

TIME STEP MANAGEMENT

Integration in cfSolutionMonitor





Optimization of time stepping strategy within the cfSolutionMonitor

BUOYANCY DRIVEN TURBULENT FLOW

General formulation

- k-ω Shear Stress Transport (SST) turbulence model (`cfKOmegaSST`):
  - blends between k-ω (near wall) and k-ε (bulk region) models (insensitive of y^+)
  - Transport of turbulent kinetic energy ***k***:

$$\frac{\partial(\rho k)}{\partial t} + \nabla\cdot\left(\rho\vec{U}k\right) = \nabla\cdot\left[\rho\left(\nu+\frac{\nu_t}{\sigma_k}\right)\nabla k\right] + P_k + P_{k,b} - \beta^*\rho\omega k + S_k$$

  - Transport of turbulent eddy frequency ***ω***:

$$\frac{\partial(\rho\omega)}{\partial t} + \nabla\cdot\left(\rho\vec{U}\omega\right) = \nabla\cdot\left[\rho\left(\nu+\frac{\nu_t}{\sigma_\omega}\right)\nabla\omega\right] + P_\omega + P_{\omega,b} - \beta\rho\omega^2 + 2\left(1-F_1\right)\ldots$$

  - Eddy viscosity ν_t:

$$\nu_t = \frac{a_1 k}{\max(a_1\omega, SF_2)}$$

  - Coefficients: $\phi = \phi_1\cdot F_1 + \phi_2\cdot(F_1 - 1)$

```
// Turbulent kinetic energy equation
tmp<fvScalarMatrix> kEqn
(
    fvm::ddt(alpha, rho, k_)
  + fvm::div(alphaRhoPhi, k_)
  - fvm::laplacian(alpha*rho*DkEff(F1), k_)
 ==
    alpha()*rho()*Pk(G)
  - fvm::SuSp((2.0/3.0)*alpha()*rho()*divU, k_)
  + PkBbyNut_.internalField()*nut()
  - fvm::Sp(alpha()*rho()*epsilonByk(F1, F23), k_)
  + kSource()
  + fvModels.source(alpha, rho, k_)
);
```

containmentFoamLibs/momentumTransport/cfKOmegaSST/cfKOmegaSSTBase.C

📖 https://turbmodels.larc.nasa.gov/sst.html

BUOYANCY DRIVEN TURBULENT FLOW

Buyoancy turbulence production and dissipation

- Buoyancy turbulence production and dissipation:
  - Simple Gradient Diffusion Hypothesis (SGDH)

$$P_{k,b} = -\frac{\nu_t}{\sigma_\rho \rho}\nabla\rho\cdot\left(\nabla p + \rho_\infty g\right) \approx -\frac{\nu_t}{\sigma_\rho}\vec{g}\cdot\nabla\rho$$

  - Generalized Gradient Diffusion Hypothesis (GGDH)

$$P_{k,b} = -\frac{3}{2}\frac{\nu_t}{\sigma_t \rho k}\left(\tau_{ij}\cdot\nabla\rho\right)\left(\nabla p + \rho_\infty \vec{g}\right)$$

$$\approx -\frac{3}{2}\frac{\nu_t}{\sigma_t \rho k}\left(\nu_t\cdot\left(\nabla\vec{U} - \nabla\vec{U}^T\right) - \frac{2}{3}k\delta_{ik}\right)\left(\vec{g}\cdot\nabla\rho\right)$$

  - Dissipation term

$$P_{\omega,b} = \nu_t\left[\left(\gamma_1 + 1\right)C_{3e}\cdot\max\left(P_{k,b},0\right) - P_{k,b}\right]$$

$$C_{3e} = C_3\cdot\tan\left(\angle\left(\vec{U},\vec{g}\right)\right)$$

containmentFoamLibs/momentumTransport/cfKOmegaSST/cfKOmegaSSTBase.C

```
template<class MomentumTransportModel, class BasicMomentumTransportModel>
void
cfKOmegaSST<MomentumTransportModel, BasicMomentumTransportModel>::
updateBuoyancyProduction()
{
    const uniformDimensionedVectorField& g_ =
        this->mesh_.objectRegistry::template
        lookupObject<uniformDimensionedVectorField>("g");

    if (buoyancyModel_ == "SGDH")
    {
        PkBbyNut_ = -1.0*(g_ & fvc::grad(this->rho_))/this->sigmaRho_;
    }

    else if (buoyancyModel_ == "GGDH")
    {
        tmp<volTensorField> tgradU = fvc::grad(this->U_);

        Info<< "### beta feature GGDH for buoyancy terms active, use with caution ###" << endl;

        PkBbyNut_ = 3.0/(2.0*this->sigmaRho_*max(this->k_,this->kMin_)) *
                (
                    g_ &
                    (
                        (this->nut_*twoSymm(tgradU)-(2.0/3.0)*this->k_*tensor::I)
                        &
                        fvc::grad(this->rho_)
                    )
                );
        tgradU.clear();
    }
```

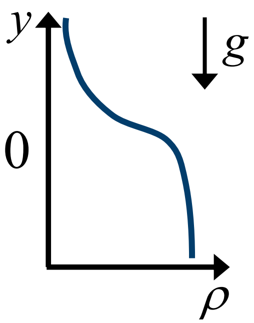
BUOYANCY DRIVEN TURBULENT FLOW

Buyoancy turbulence production and dissipation

- Buoyancy forces can suppress or enhance turbulent fluctuations:
  - Stably stratified flow
  - Unstably stratified flow

Stably stratified flow

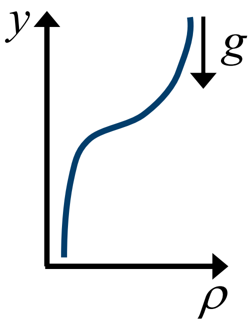
$$\partial\rho / \partial y < 0$$



$$P_{k,b} \sim -\vec{g} \cdot \nabla\rho < 0$$

Unstably stratified flow

$$\partial\rho / \partial y > 0$$



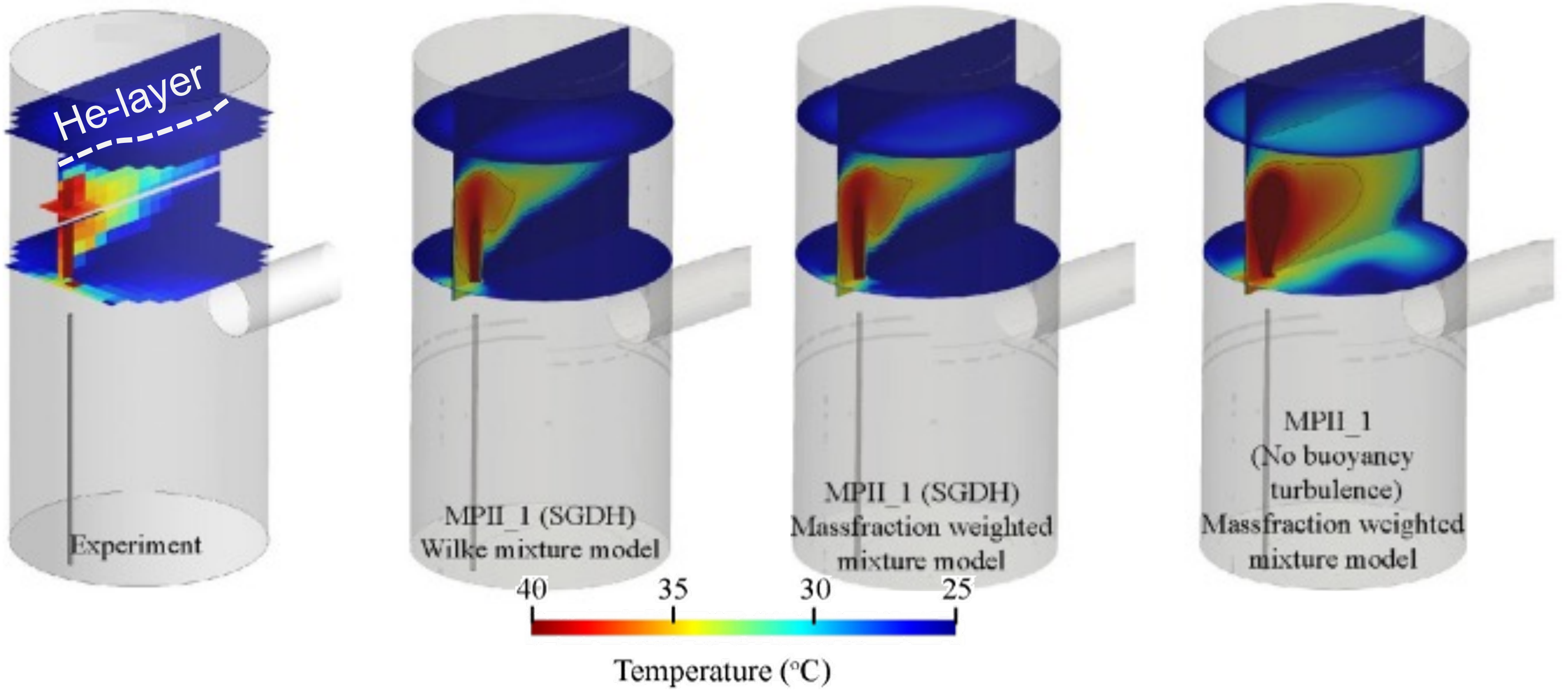
$$P_{k,b} \sim -\vec{g} \cdot \nabla\rho > 0$$

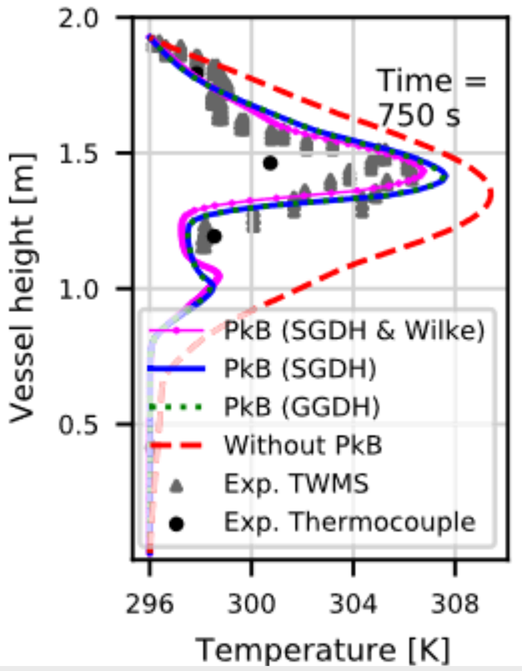
➢ In mixed and free convection flows, $P_{k,b}$ can be in the order of P_k and must not be neglected !

BUOYANCY DRIVEN TURBULENT FLOW

Validation - MiniPanda

- MiniPanda MPII_1 experiment: Mixing of a stably stratified Helium layer by a vertical jet (here t=750s)





MPII_1 experiment sim. vs. exp.
figure from Kampili. et al., 2021

➢ Visible effects of buoyancy terms, but less for material properties and model formulation

📖 M. Kampili. et al., "CFD simulations of stratified layer erosion in MiniPanda facility using the tailored CFD solver containmentFOAM", IJHMT 178 (2021) 121568

WALL CONDENSATION

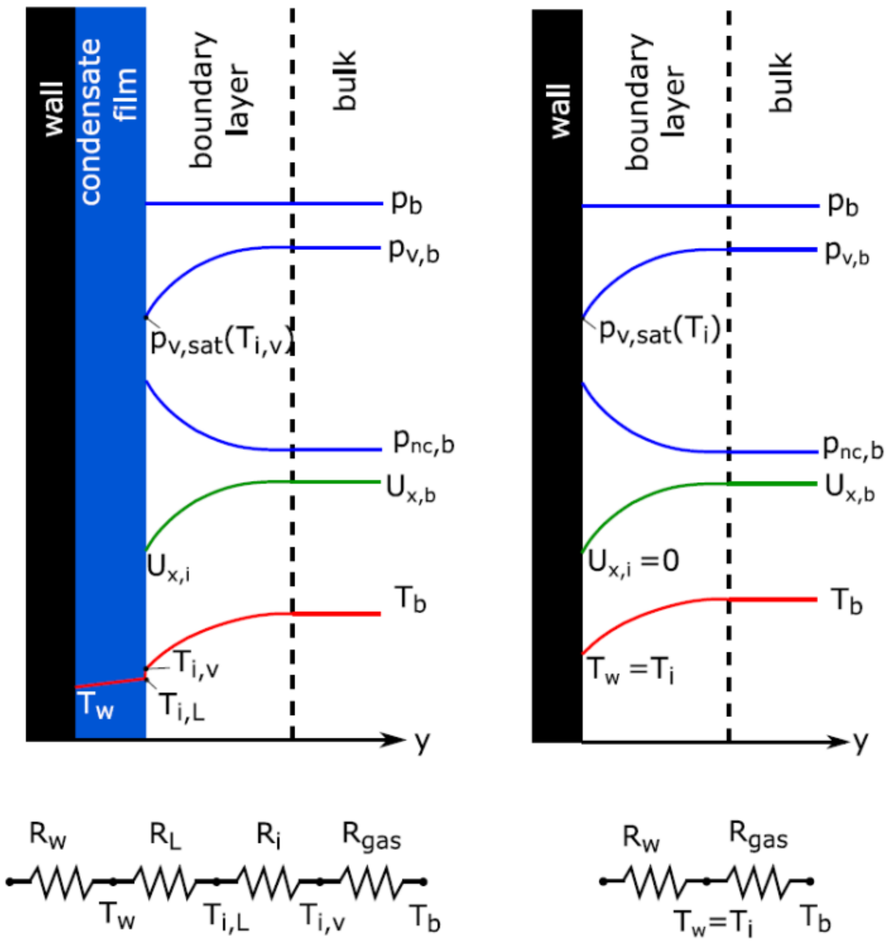
Model

- Wall condensation – modeling assumptions:
  - Impermeable condensation interface (Stefan's approach)
  - Arbitrary multi-component mixtures
  - No interfacial thermal resistance $T_{i,V} = T_{i,L}$
  - Thin and stagnant film, $T_i = T_w$, $U_{\parallel,i} = 0$ m/s

➢ The liquid phase can be omitted and the condensation rate is determined by the mass transport in the boundary layer

$$\dot{m}''_{i,v} = \frac{1}{1-Y_{v,i}} \rho \left(D_{v,m} + D_t \right) \frac{\partial Y_v}{\partial y} \bigg|_w$$

➢ Challenge: Modeling the resistance of the boundary layer D_t



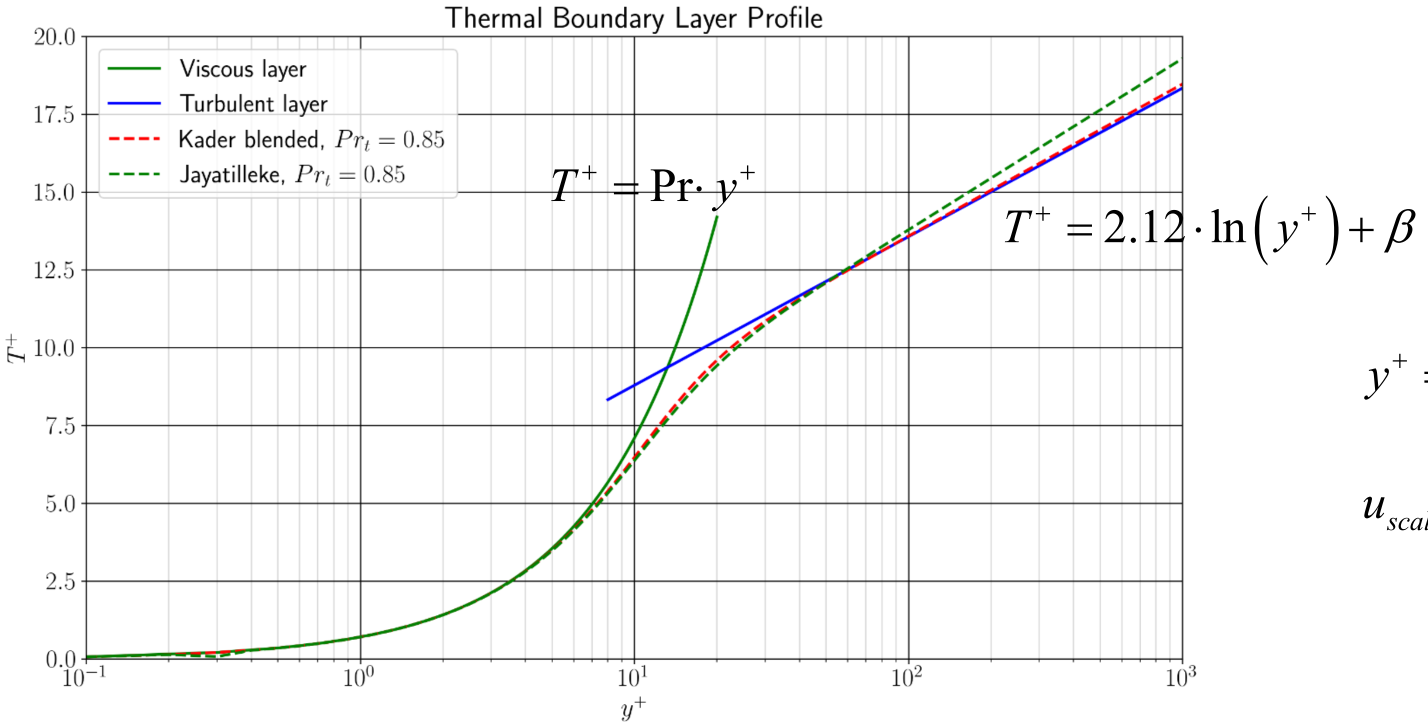
Physics vs. modeling of wall condensation, figure from Vijaya Kumar G. et al., 2021

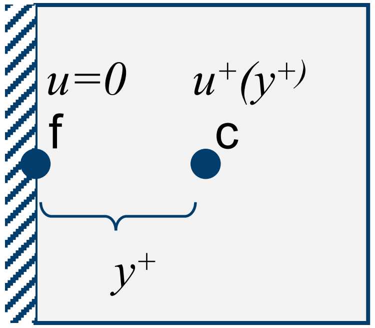
📖 Vijaya Kumar G. et al., "Implementation of a CFD model for wall condensation in the presence of non-condensable gas mixtures," Applied Thermal Engineering, 116546, 2021

WALL CONDENSATION

Wall function concept

- Idea: Link known face values (Dirichlet BC) to cell values for an arbitrary boundary mesh resolution
  - use predefined scalable variable profiles, e.g., $u^+(y^+)$, $T^+(y^+)$, $Y_s^+(y^+)$, ..
  - to evaluate the turbulent diffusivity (ν_t, α_t, $D_{t,i}$ ..) in the near wall cell and yield an ideally mesh independent boundary flux





$$y^+ = \frac{u_{scale} y}{\nu}$$

$$u_{scale}: \quad u_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad or \quad u^* = C_\mu^{0.25}\sqrt{k}$$

WALL CONDENSATION

Wall treatment in containmentFOAM

- Definition of a baseline set of continuous wall functions:

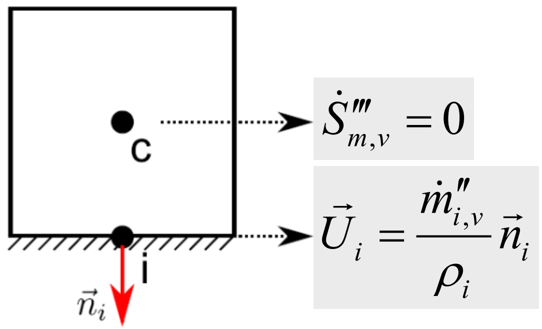
equation	layer-wise formulation	blended + non-equilibrium factor	
Momentum (streamwise)	sub-layer: $u_l^+ = y^+$ log-layer: $u_t^+ = \frac{1}{0.41}\ln y^+ + 5.2$	$u^+ = \sqrt[4]{\left(1/u_l^{+4} + 1/u_t^{+4} \right)^{-1}}$	(nutUSpaldingFOWallFunction)
Energy (Kader, 1981)	sub-layer: $T_l^+ = \Pr \cdot y^+$ log-layer: $T_t^+ = 2.12\ln y^+ + \beta(\Pr)$ $\beta(\Pr) = \left(3.85\Pr^{1/3} - 1.3\right)^2 + 2.12\ln \cdot (\Pr)$	$T^+ = \sqrt[4]{\left(1/T_l^{+4} + 1/T_t^{+4} \right)^{-1}}$	(alphatKaderWallFunction)
Steam mass fraction (Kader, 1981)	sub-layer: $Y_{S,l}^+ = Sc \cdot y^+$ log-layer: $Y_{S,t}^+ = 2.12\ln y^+ + \beta(Sc)$ $\beta(Sc) = \left(3.85Sc^{1/3} - 1.3\right)^2 + 2.12 \cdot \ln(Sc)$	$Y_S^+ = \sqrt[4]{\left(1/Y_{S,l}^{+4} + 1/Y_{S,t}^{+4} \right)^{-1}}$	(DtKaderWallFunction)
Turbulence (Menter 2003) Turbulence eddy frequency	sub-layer: $\omega_l = \frac{6 \cdot \nu}{\beta(\Delta y)^2}$ log-layer: $\omega_t = \frac{u_\tau^2}{a_1 \kappa \nu y^+}$	$\omega = \omega_l \sqrt{1 + \left(\frac{\omega_l}{\omega_s}\right)^2}$	(omegaMenterWallFunction)
Turbulence kinetic energy	$\partial k / \partial y = 0$		(zeroGradient)

WALL CONDENSATION

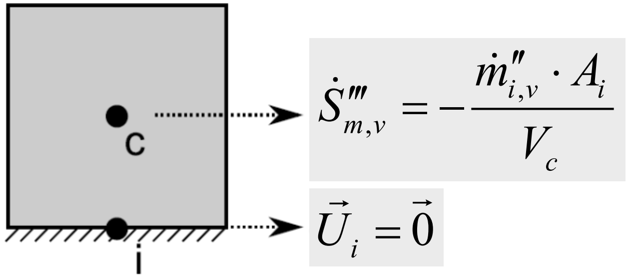
Model implementation

- Model implementation:

Face-flux



Volumetric source terms



- preferred option, less grid sensitive
- quantities (h, k, ω ..) associated with condensate are implicitly removed by face flux
- Boundary conditions:
  - $Y_{i,v}=p_{sat}(T_i)$, $Y_{nc,i}=f(D_{eff}, U_{i,\perp})$

- direct approach in most commercial codes
- often requires separate sink terms for associated quantities
- Boundary conditions:
  - $Y_{nc,i}=p_{sat}(T_i)$, $\partial Y_{nc,i}/\partial y = 0$

- D_t, α_t: Kaders' wall function
- ν_t: Spalding wall function
- T: latent heat flux added to wall heat balance (CHT, Robin, von Neumann) or omitted (Dirichlet)

📖 Vijaya Kumar G. et al., "Implementation of a CFD model for wall condensation in the presence of non-condensable gas mixtures," Applied Thermal Engineering, 116546, 2021

WALL CONDENSATION

Implementation

- containmentFoamLibs/condensation/

```
└── wallCondensation
    ├── DtJayatilleke
    │   ├── DtJayatilleke.C
    │   └── DtJayatilleke.H
    ├── DtKader
    │   ├── DtKader.C
    │   └── DtKader.H
    ├── noWallCondensation
    │   ├── noWallCondensation.C
    │   └── noWallCondensation.H
    ├── wallCondensationBase.C
    └── wallCondensationBase.H
```

wall functions

base class (wallCondensationBase ::updateCondensation MassFlux())

WALL CONDENSATION

How to use it ?

- 0/boundaryFields

Variable	Boundary Condition	Options
T	fixedValue	HTC, CHT
U	condensingWallVelocity	
alphat	alphatKaderWallFunciton	
k	zeroGradient	
nut	nutUSpaldingFOWallFunction	
omega	omegaMenterWallFunction	
p_rgh	fixedFluxPressure	
p	calculated	
H2O	saturatedSteam	
inertSpecie	calculated	
nonCondensables	nonCondensableMassFraction	speciesName

- constant/condensationProperties

```
velocityScale        blendedUStar;
DtWallFunction       DtKader;

Sct_wall             0.7;
```

blendedUStar (default); optional uTau, uStar

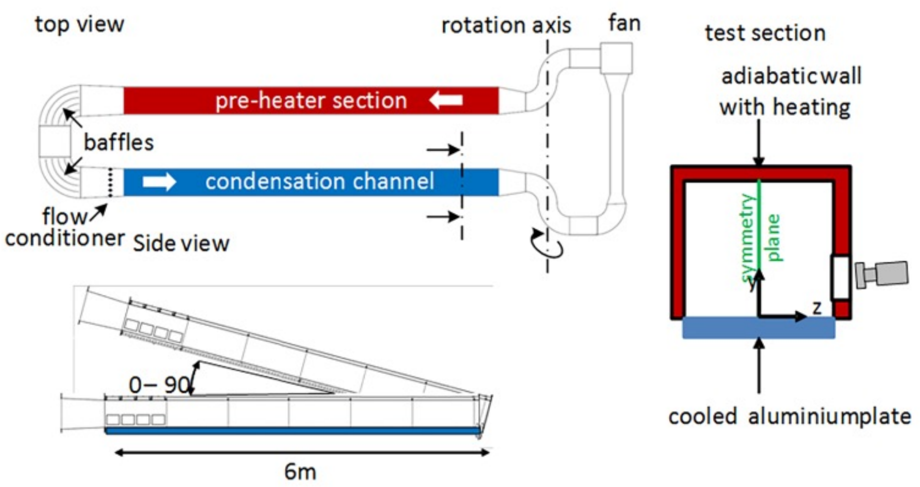
DtKader (default), DtJayatilleke

Sc_t in the near wall cell

WALL CONDENSATION

Validation - SETCOM

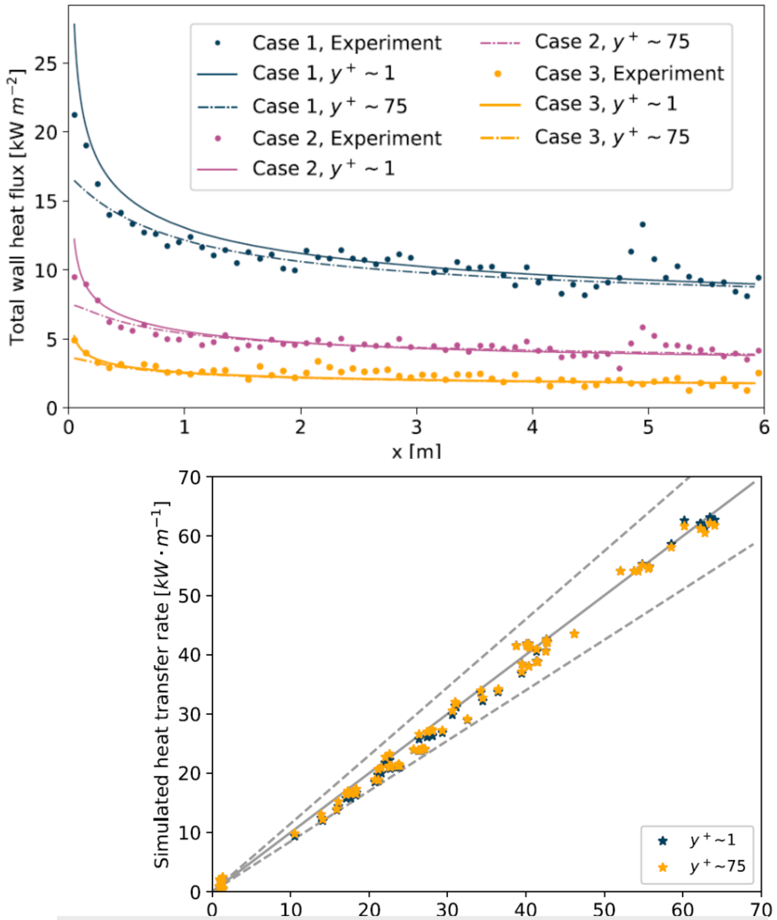
- Model V&V:
  - Separate Effect Test for Condensation Modeling (SETCOM)



S. Kelm et al., "Development of a multi-dimensional wall-function approach for wall condensation," Nuclear Engineering and Design, 353 (110239), 2019

➢ Reasonable prediction of condensation rate for low-Re meshes possible

➢ If wall functions are used, the error increases with deviation from their underlying modeling assumptions (no buoyancy, pressure gradients or suction..)



Forced convection condensation heat transfer, figure from Vijaya Kumar G. et al., 2021

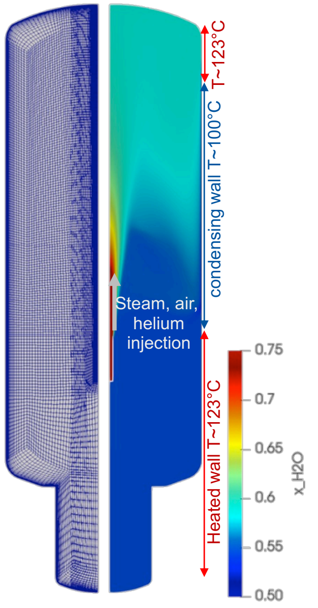
WALL CONDENSATION

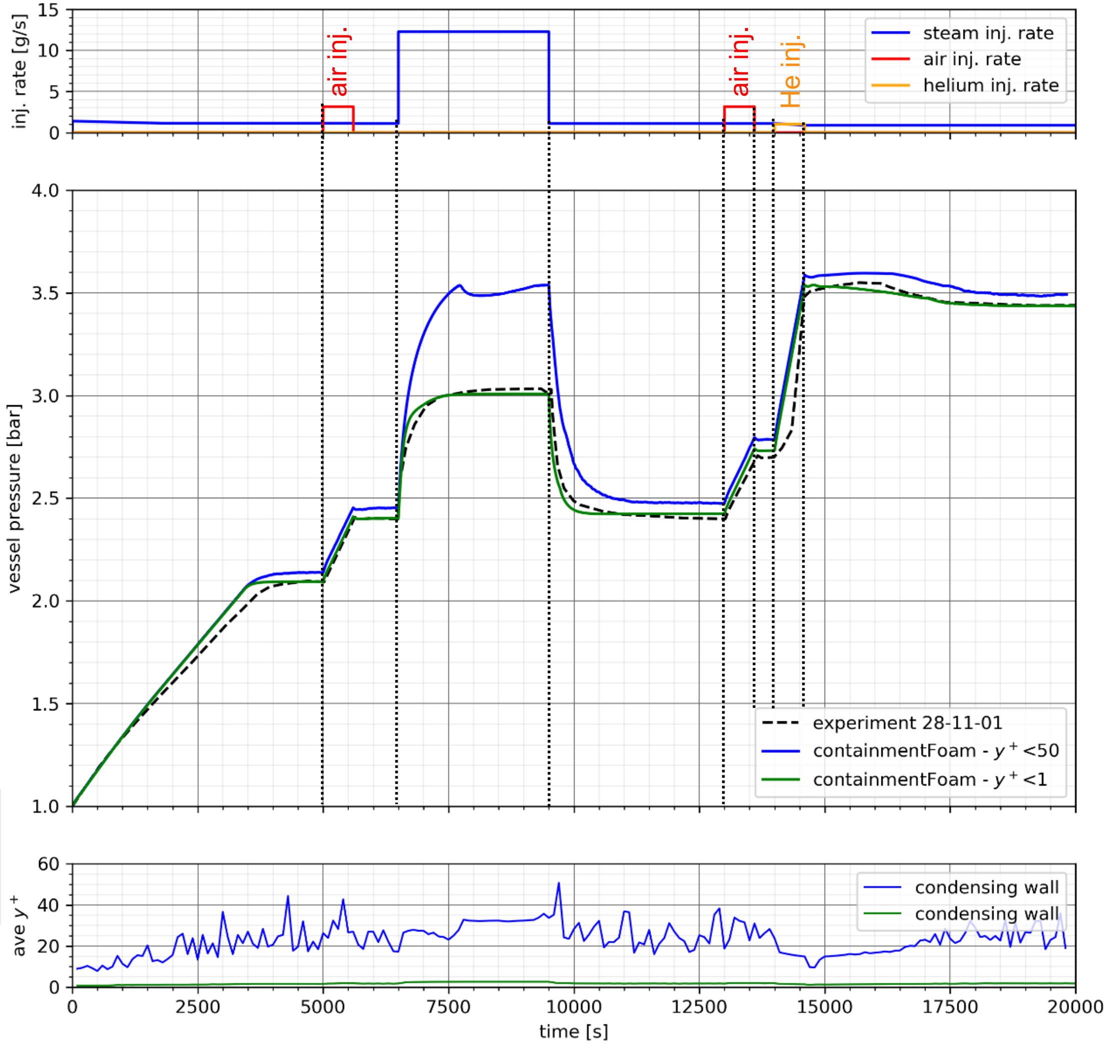
Validatio – ISP47 TOSQAN

- Model V&V:
  - ISP-47 on containment thermal hydraulics
  - TOSQAN (7m³) tests
    - 🕮 Malet et al. Nuclear Engineering and Design 240 (2010) 3209–3220

➢ Reasonable prediction of transient pressure evolution possible, but

➢ standard wall functions tend to under predict the condensation rate (→ higher pressure)





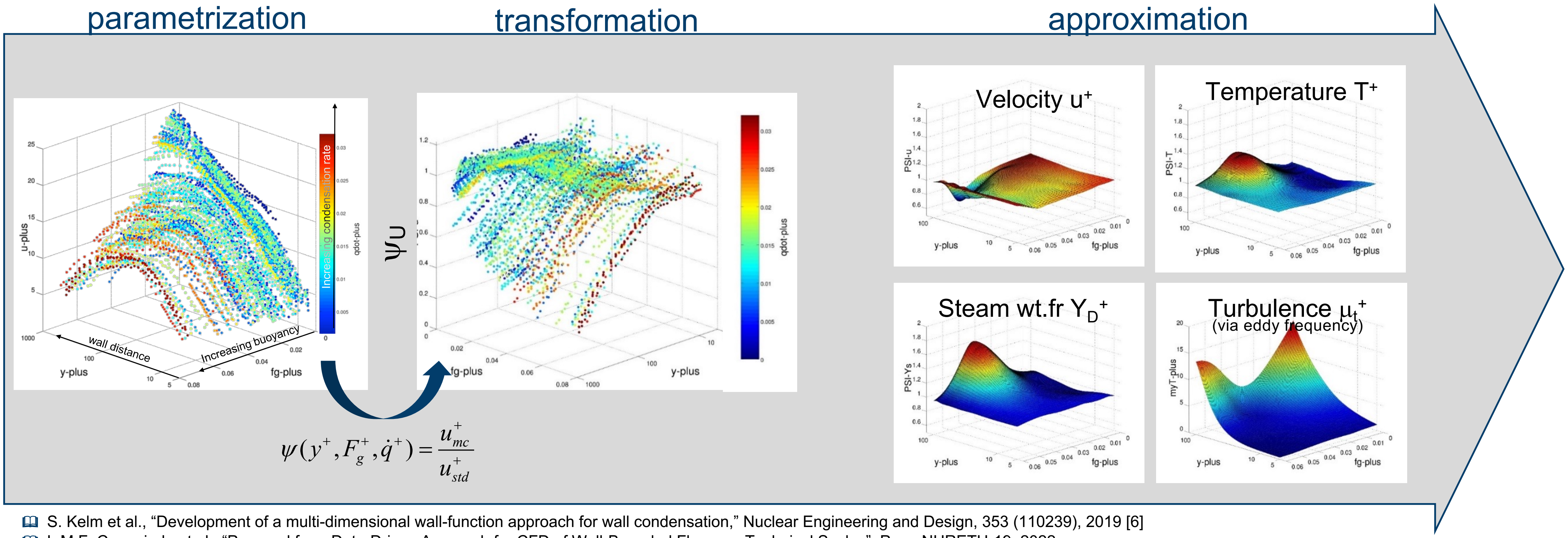
TOSQAN-ISP 47 scenario (l) and pressurization transient (r), own figure

WALL CONDENSATION

WIP – Improved wall treatment

WIP

- Wall functions – Mixed Convection (work-in-progress)
  - Data-driven approach



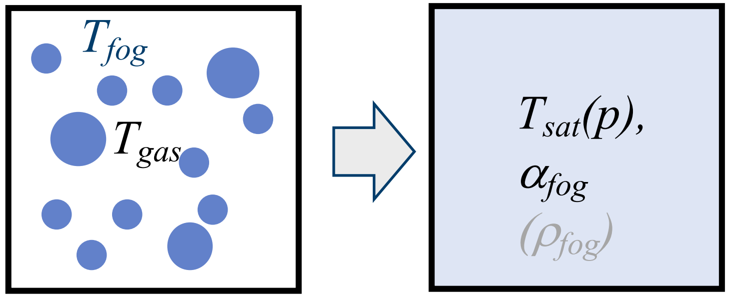
📖 S. Kelm et al., “Development of a multi-dimensional wall-function approach for wall condensation,” Nuclear Engineering and Design, 353 (110239), 2019 [6]

📖 L.M.F. Cammiade et al., “Proposal for a Data-Driven Approach for CFD of Wall-Bounded Flows on Technical Scales”, Proc. NURETH-19, 2022

BULK CONDENSATION AND FOG TRANSPORT

Model

- Bulk condensation – modeling assumptions:
  - Thermal equilibrium ($T_{fog}=T_{gas}$)
  - Infinitesimally fast nucleation processes
  - Constant fog droplet diameter



➢ Bulk condensation rate is obtained from *'return to saturation in constant time scale'*

📖 L. Vyskocil. et al., "CFD simulation of air–steam flow with condensation", Nuclear Engineering and Design 279 (2014)

$$\dot{S}'''_{fog,m} = \frac{\dot{S}'''_{fog,e}}{h_{lat}}$$

$$\dot{S}'''_{fog,e} = \frac{1}{\Delta t}\begin{cases} \min\left[\rho c_p\left(T_{sat}(p_{steam})-T\right),\ \rho Y_{steam} h_{lat}\right] & \textit{if condensing: } T_{sat}(p_v)>T \\ \max\left[\rho c_p\left(T_{sat}(p_{steam})-T\right),\ -\rho_{fog} h_{lat}\right] & \textit{if evaporating: } T_{sat}(p_v)<T \end{cases}$$

➢ Fog transport is considered using a passive scalar drift flux approach in an Eulerian framework

📖 E.M.A. Frederix et al., "Eulerian modeling of inertial and diffusional aerosol deposition in bent pipes", Computers and Fluids 159 (2017), pp 217 – 231

credits to A. George

BULK CONDENSATION AND FOG TRANSPORT

Model

- Model implementation:
  - Drift flux transport equation (α_{fog}: fog volume fraction)

$$\frac{\partial(\alpha_{fog})}{\partial t} + \nabla \cdot \left[\alpha_{fog}\left(\vec{U} + \vec{U}_{drift}\right)\right] = \nabla \cdot \left[\left(D_{Brownian} + \frac{\nu_t}{Sc_t}\right)\nabla \alpha_{fog}\right] - \frac{\dot{S}'''_{fog,m}}{\rho_{fog}}$$

convection & drift due to forces | Brownian & turbulent diffusion | condensation & evaporation

- Drift: Stokes and simplified Manninen model

$$\frac{\partial\left(\vec{U}_{drift}\right)}{\partial t} + \left(\vec{U}_{drift} \cdot \nabla\right) \cdot \vec{U}_{drift} = -\frac{\left(\vec{U}_{drift} - \vec{U}\right)}{\tau_{fog}} + \frac{\left(\rho_{fog} - \rho_{gas}\right)}{\rho_{fog}}\vec{g};$$

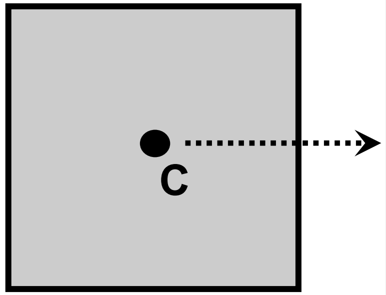
$$\tau_{fog} = \frac{\rho_{fog} d_{fog}^2}{18\mu}$$

- Brownian Diffusion (Stokes-Einstein model)

$$D_{Brownian} = \frac{k_B C_c T}{3\pi\mu d_{fog}}$$

➢ Droplet diameter impacts settling

volumetric source terms



$$\dot{S}'''_{fog,m}$$

$$\dot{S}'''_{v,m} = -\dot{S}'''_{fog,m}$$

$$\dot{S}'''_{fog,h} = \dot{S}'''_{fog,e} - \dot{S}'''_{fog,m} c_{p,v} T$$

$$\dot{S}'''_{fog,U} = -\dot{S}'''_{fog,m} \vec{U}$$

$$\dot{S}'''_{fog,k} = -\dot{S}'''_{fog,m} k$$

$$\dot{S}'''_{fog,\omega} = -\dot{S}'''_{fog,m} \omega$$

📖 A. George, S. Kelm, H.J. Allelein, “Efficient CFD Modeling of Bulk Condensation, Fog Transport and Re-Evaporization for Application to Containment Scale, Nuclear Engineering and Design Volume 401, January 2023, 112067

credits to A. George

BULK CONDENSATION AND FOG TRANSPORT

Size distribution

WIP

- Population Balance Modeling
  - Fog size distribution is discretized in i volume intervals (Δv_i) (i typically < 10)
  - Drift flux transport equation for interval i volume fraction ($\alpha_i = N_i v_i$)

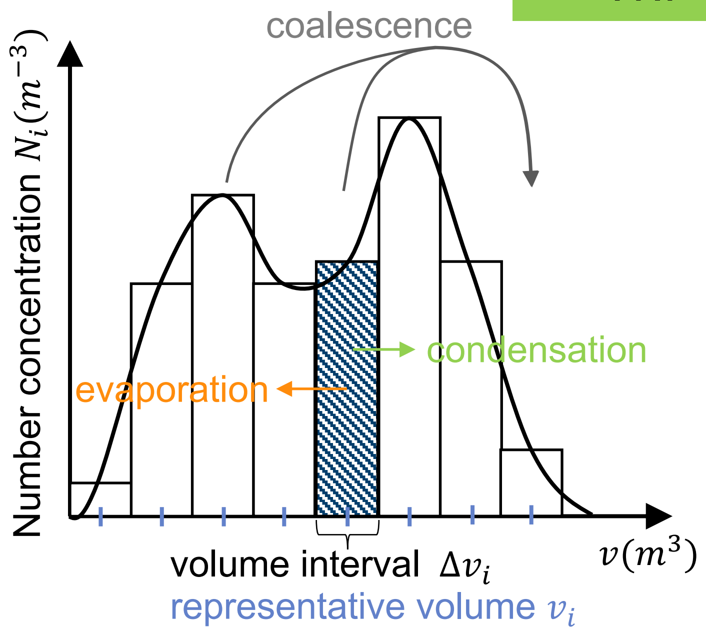
$$\frac{\partial(\alpha_i)}{\partial t} + \underbrace{\nabla \cdot \left[\alpha_i \left(\vec{U} + \vec{U}_{drift,i}\right)\right]}_{\text{convection \& drift (e.g. settling)}} = \underbrace{\nabla \cdot \left[\left(D_{Brownian,i} + \frac{\nu_t}{Sc_t}\right)\nabla \alpha_i\right]}_{\text{Brownian \& turbulent diffusion}} - \underbrace{\frac{\dot{S}_i'''}{\rho_{fog}}}_{\text{condensation into \& evaporation from group i, as well as coalescence}}$$

convection & drift (e.g. settling)

Brownian & turbulent diffusion

condensation into & evaporation from group i, as well as coalescence

  - Size change due to
    - condensation / evaporation
    - coalescence (breakup no considered)



Population Balance modeling, figure by openfoam.org

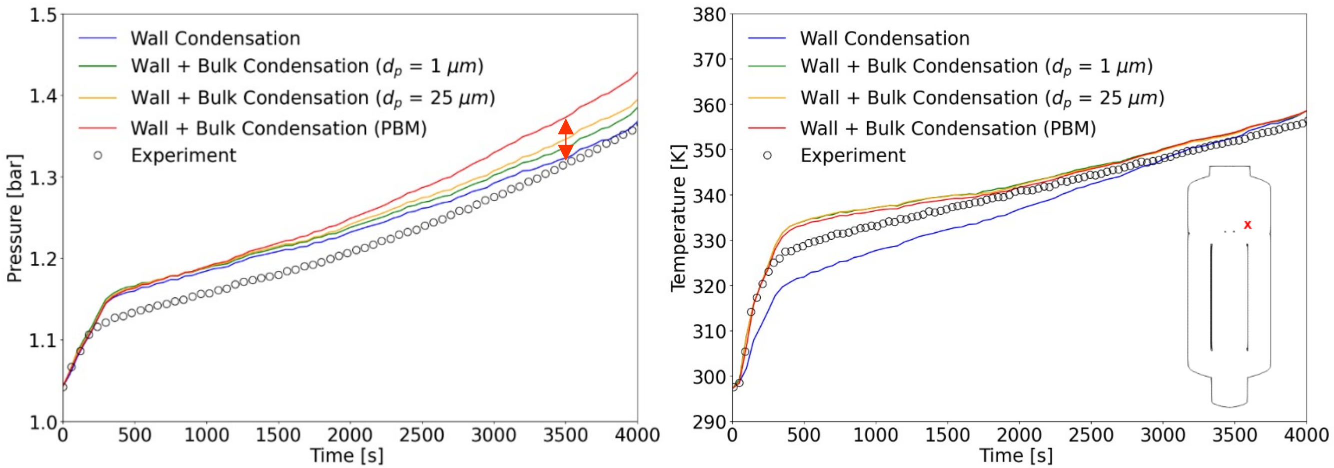
openfoam.org/guides/population-balance-modelling

credits to A. George

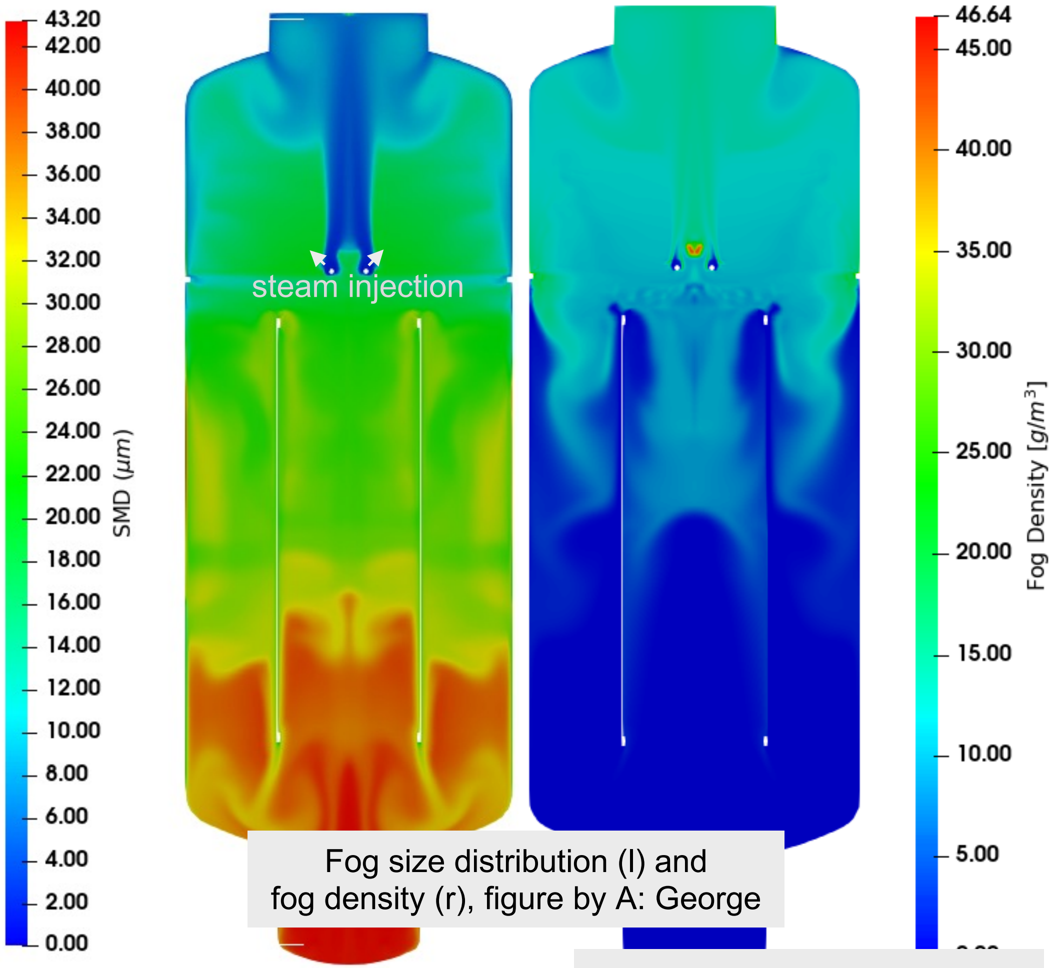
BULK CONDENSATION AND FOG TRANSPORT

Validation

- THAI-TH2 Experiment: Steam injection into cold THAI facility:



Effect of fog formation on pressure (l) and gas temperature (r), figure by A: George



Fog size distribution (l) and fog density (r), figure by A: George

> ➢ Major relevance of bulk condensation is not given by water/steam balance itself, but by its interactions

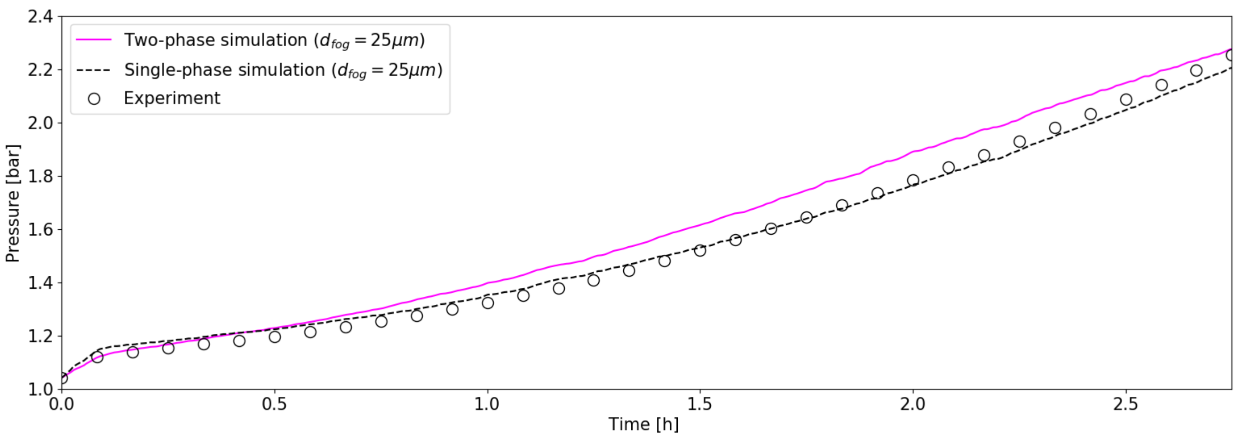
A. George, S. Kelm, H.J. Allelein, "Efficient CFD Modeling of Bulk Condensation, Fog Transport and Re-Evaporization for Application to Containment Scale, Nuclear Engineering and Design Volume 401, January 2023, 112067

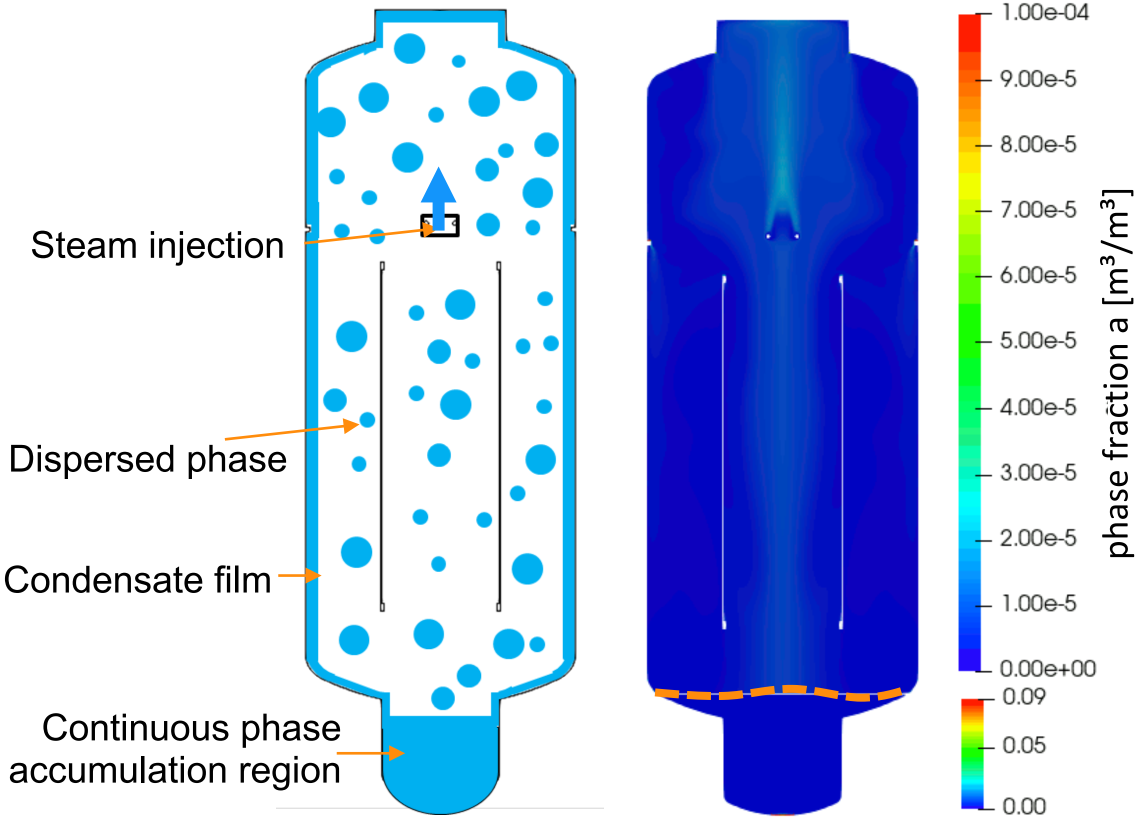
credits to A. George

PERSPECTIVES

SMR Applications - VOF modelling for (multi-component) gas and water phase

- Mixture momentum equation
- Drift flux approach for relative motion of fog droplets due to inertia, gravity, drag and diffusion
- Thermal non-equilibrium between phases
- Bulk, wall and interface condensation





THAI TH2 experiment

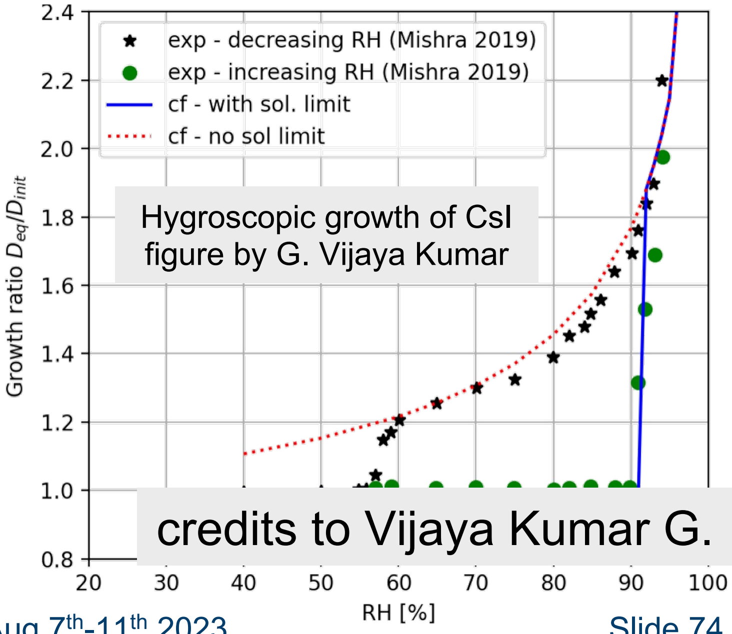
credits to A. George

FOG AND AEROSOL TRANSPORT

Phenomenology

- Containment: primarily fog but also radioactive substances
- Single phase – drift flux approach
  - Transport:
    - Passive scalar transport equation
    - Thermal equilibrium
    - Forces: drag, gravity, thermo-, turbo-, diffusiophoresis.
  - Size variation and distribution:
    - Hygroscopic growth, condensation & evaporation, (de-)agglomeration
    - Sectional approach

$$\frac{\partial(\rho_{fog})}{\partial t} + \underbrace{\nabla \cdot \left[\rho_{fog}\left(\vec{U} + \vec{U}_{drift}\right)\right]}_{\text{convection \& drift due to forces}} = \underbrace{\nabla \cdot \left[\left(D_{Brownian} + \frac{\nu_t}{Sc_t}\right)\nabla \rho_{fog}\right]}_{\text{Brownian \& turbulent diffusion}} - \underbrace{\dot{S}'''_{fog,m}}_{\text{condensation \& evaporation}}$$



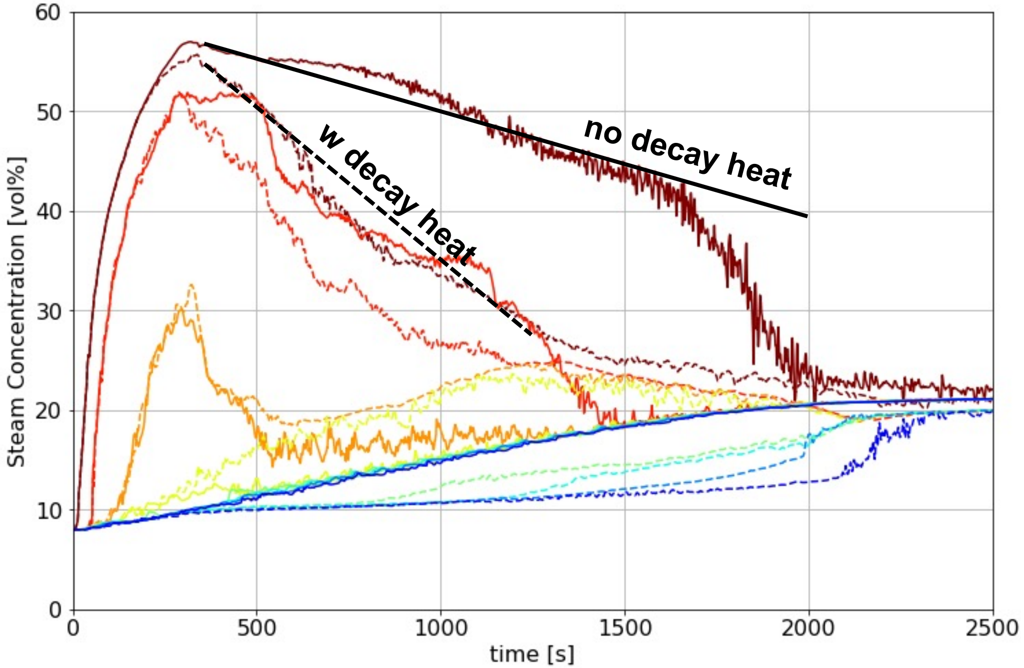
credits to Vijaya Kumar G.

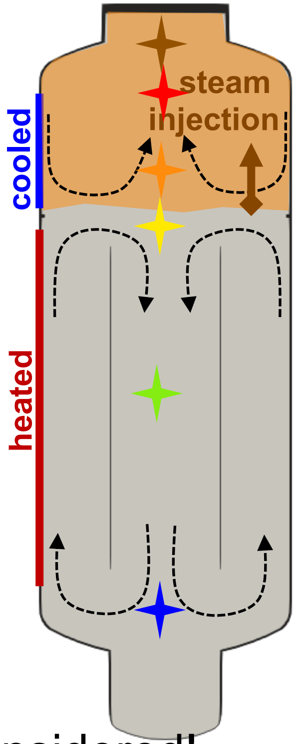
G. Vijaya Kumar, "CFD Simulation of the Interaction of Buoyant Flows with Nuclear Aerosols", PhD thesis RWTH Aachen University and IITM Madras, December 2022

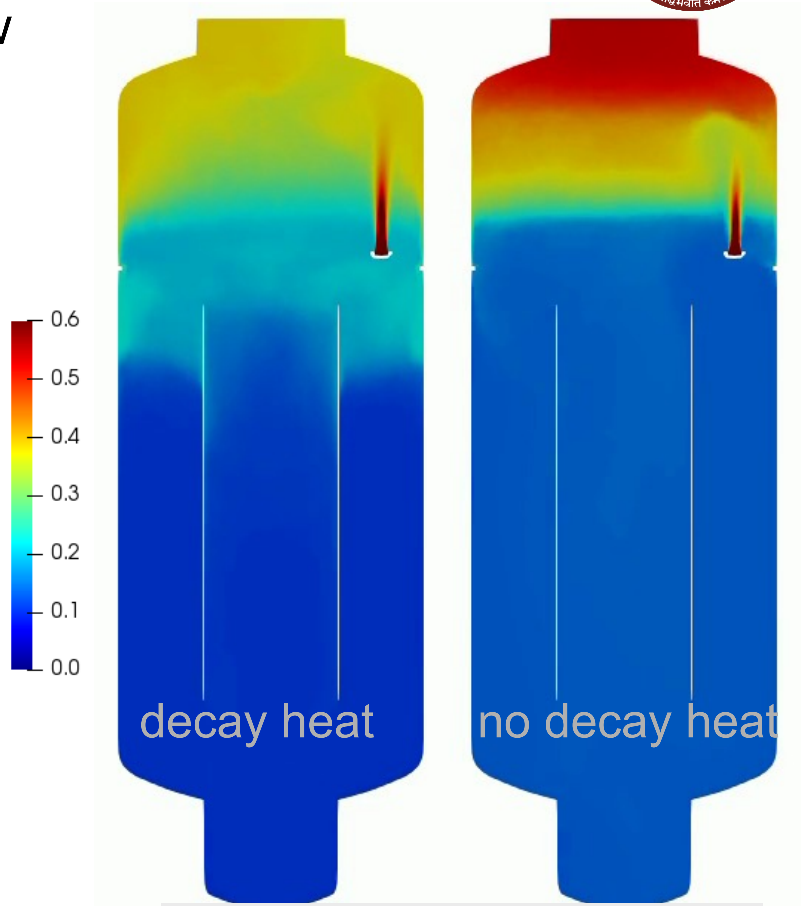
FOG AND AEROSOL TRANSPORT

Impact of airborne decay heat

- Scoping analysis to investigate the impact on a buoyancy driven flow
  - THAI-TH24: Injection of 60 g CsI along with steam







credits to Vijaya Kumar G.

➢ Significantly different mixing behavior if decay heat is considered!

📖 G. Vijaya Kumar, "CFD Simulation of the Interaction of Buoyant Flows with Nuclear Aerosols", PhD thesis RWTH Aachen University and IITM Madras, December 2022

AEROSOL TRANSPORT

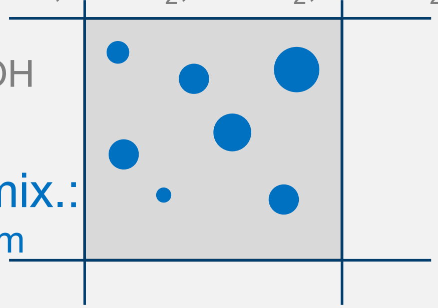
Aerosol library - Refactoring

WIP

- Status: Harmonization of bulk condensation and fog transport models required
  - Forces: Drag, gravity, thermo-, diffusion-, turbophoresis
  - Mass transfer: Nucleation, bulk condensation and evaporation incl. hygroscopic growth
  - Aerosol size distribution: moment method, sectional approach, mono-dispersed

➢ Approach: Integrating fog as sub model into the aerosol library

gas mixture:
- 65% steam, 5% H_2, 5% O_2, 20% N_2
- 6 % CsI
- 4% NaOH



aerosol mix.:
- 95% steam
- 2 % CsI
- 3% NaOH

mixture properties

mass transfer

single phase, drift flux approach for a passive scalar framework

- Mono dispersed
- Moment method
- Sectional approach

Size distribution

$$\frac{\partial \alpha_i}{\partial t} + \nabla \cdot \left[\alpha_i \left(\vec{U} + \vec{U}_{drift} \right) \right] = \nabla \cdot \left[\left(D_{Brownian} + \frac{\nu_t}{Sc_t} \right) \nabla \alpha_i \right] - \frac{\dot{S}'''_{\alpha_i}}{\rho_{aero}}$$

convection & drift due to forces | Brownian & turbulent diffusion | mass transfer

set of n+k passive scalar transport eqns.

credits to Vijaya Kumar G.

BULK CONDENSATION AND FOG TRANSPORT

Implementation

- containmentFoamLibs/condensation/

base class

condensation rate models

drift flux / forces

```
├── bulkCondensation
    ├── bulkCondensationBase.C
    ├── bulkCondensationBase.H
    ├── bulkCondensationBaseI.H
    ├── noBulkCondensation
    ├── VyskocilSchmidMacek
        ├── VyskocilSchmidMacek.C
        └── VyskocilSchmidMacek.H
    └── subModels
        ├── BrownianDiffusionModels
            ├── BrownianDiffusionModel
            │   ├── constantBrownian
            │   ├── noBrownian
            │   └── StokesEinstein
            └── driftModels
                ├── driftModel
                ├── IshiiMishima
                ├── Manninen
                ├── noDrift
                ├── SchillerNaumann
                └── Stokes
```

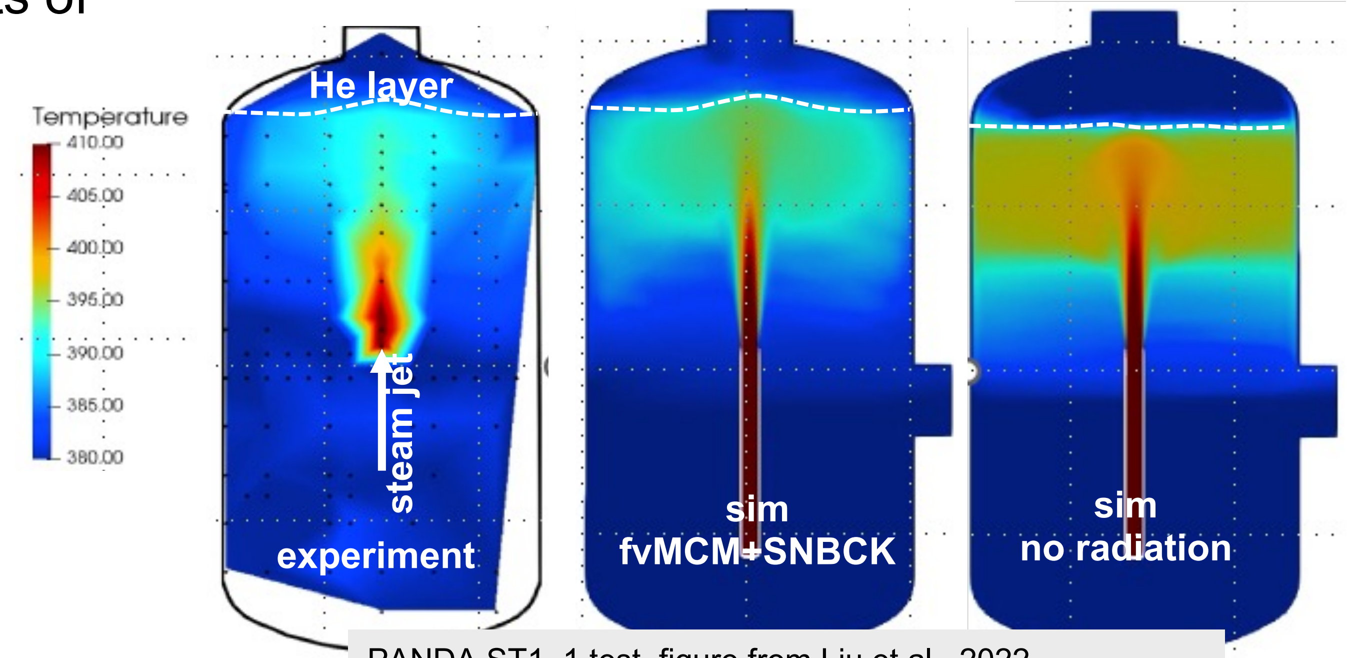
GAS RADIATION IN CONTAINMENT FLOWS

Introduction

- Radiative heat transfer ~ T^4, while T_{max}-T_{min}~$50K$
- Thermal radiation can transfer heat over distance
- and containment flows involve large stagnant gas volumes
- Containment atmosphere holds large amounts of IR active species steam, CO, CO_2
- Energy deposited in participating media introduces secondary buoyancy driven flows

- Major challenges:
  - solve the radiative transport equation
  - model the spectral properties of the medium
  - interaction with thermo-fluid dynamics

📖 X. Liu et al., "Monte Carlo method with SNBCK nongray gas model for thermal radiation in containment flows", NED 390, 111689, 2022



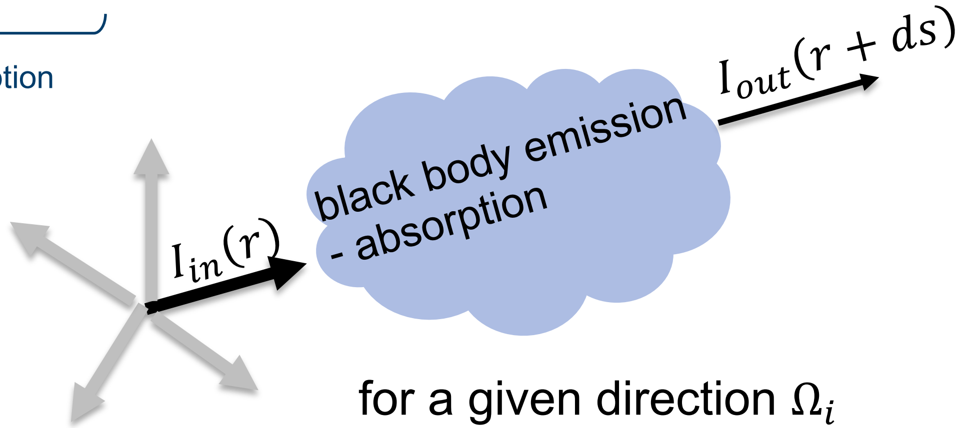
PANDA ST1_1 test, figure from Liu et al., 2022

RADIATIVE TRANSFER EQUATION

Concept

- The steady-state spectral radiative transfer equation (RTE) in a non-scattering medium is

$$\frac{dI_\eta(r,\Omega)}{ds} = \Omega \cdot \nabla I_\eta(r,\Omega) = \underbrace{\kappa_\eta I_{b,\eta}(r,\Omega)}_{\text{black body emission}} - \underbrace{\kappa_\eta I_\eta(r,\Omega)}_{\text{absorption}}$$



for a given direction Ω_i

- Beer Lambert law:

$$I_\eta(s) = I_\eta(0)\, e^{-\kappa_\eta s}$$

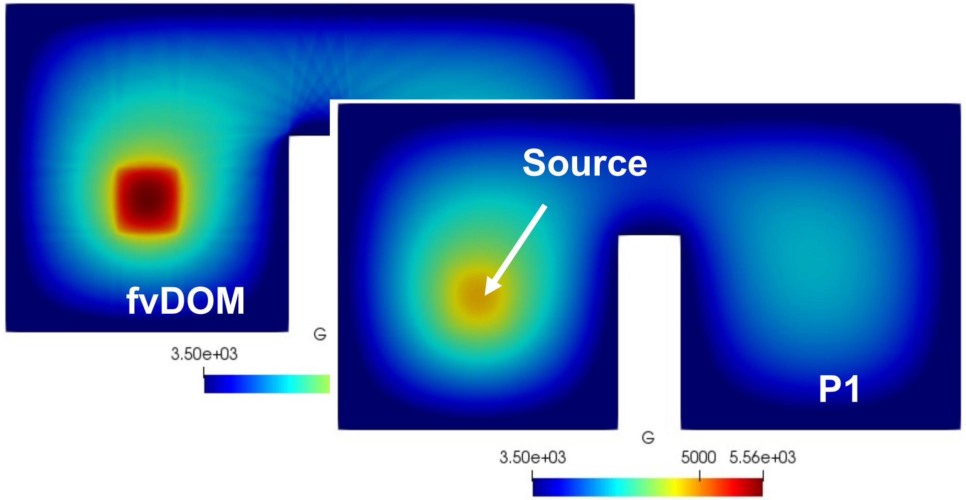
- Planck's black body emission:

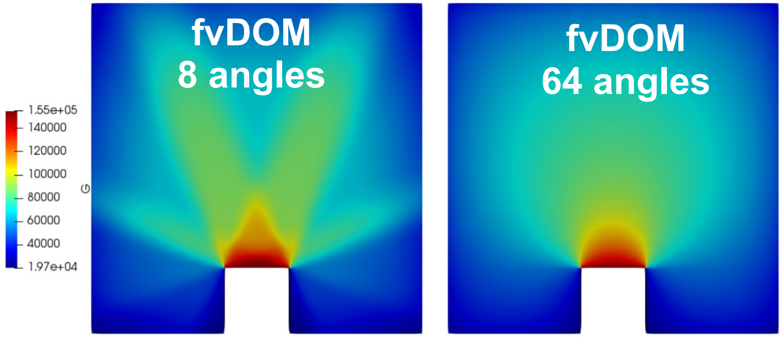
$$I_{b,\eta}(T) = \frac{2hc^2\eta^3}{e^{\frac{hc\eta}{kT}} - 1}$$

RADIATIVE TRANSFER EQUATION

Solution Methods

- 1^{st} order spherical harmonics (P_1)
  - diffusive transport equation → no directional dependency
  - only optically thick media
  - only gray spectral properties
- Discrete Ordinate Method (DOM) / S_N
  - Discretization of sphere surface into few directions → ray effect, false scattering
  - Solves differential form of RTE for each energy band
  - Expensive, in particular with non-gray properties
- Monte Carlo Method (MCM)
  - Solving integral RTE along a photon path (sampling photons with wave n
  - Error reduced with number of photon histories (→ cost!)
  - Efficient with non-gray models, geometric flexibility





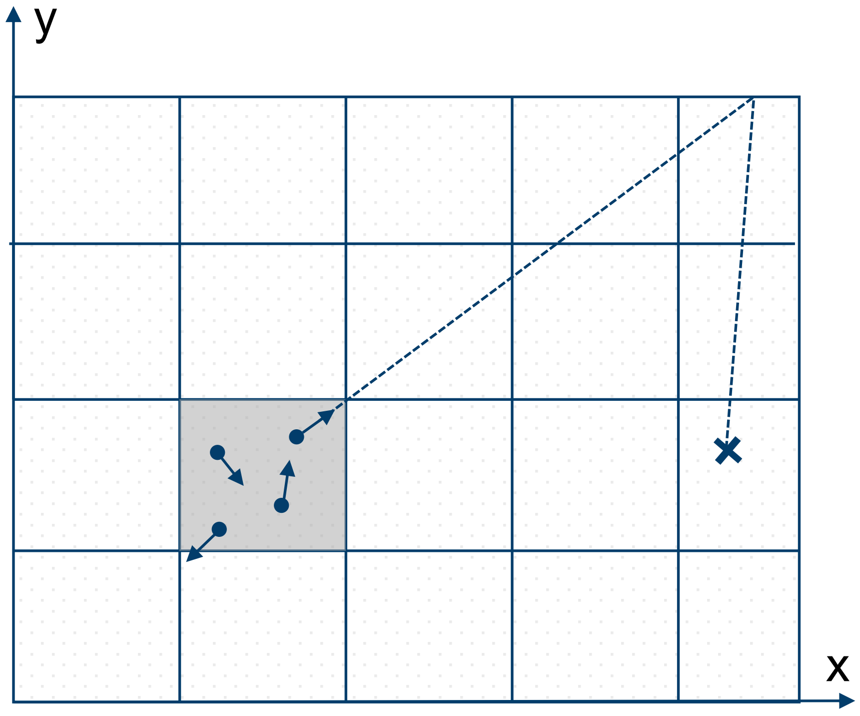
Comparison of P1 and fvDOM (top) and ray effect (bottom), figure by X. Liu

MONTE CARLO SOLVER

Radiatve Energy Absorption Distribution Monte Carlo Method Algorithm

- Built on the Lagrangian library in OpenFOAM
  - Determine the total emission energy
    - Black body $Q_{emission} = 4\,\kappa\,\sigma\,T^4\,V$
  - Sample position (x, y, z) and direction (u, v, w) of n photons per cell
  - Photon tracking along its path s
    - Beer's law $E_{out} = E_{in}\,(x, y, z;\ u, v, w)\,(1 - e^{-k(x,y,z)s})$
  - Resample photon direction if it hits a wall face
  - Compute energy deposition in each cell along the path s
    - $Q_{absorption} = \sum_n E_0(x, y, z;\ u, v, w)\,e^{-k(x,y,z)s}$
  - Continue until the photon energy is below a threshold value
  - Summarize the radiation source term
    - $-divQr = (Q_{absorption} - Q_{emission})/V$

Basic fvMCM algorithm for a gray medium, figure by X. Liu



statistical error $\sigma = \frac{S}{\sqrt{N}}$

credits to X. Liu

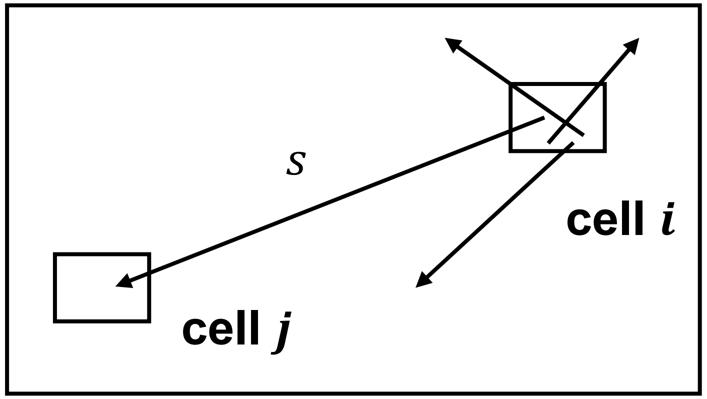
MONTE CARLO SOLVER

Monte Carlo Solver Efficiency Improvement: Algorithm Improvements

- Monte Carlo method (`standard`)
  - Statistical error due to the finite number of directions/photons
  - Hard to reduce fluctuations in complex 3D geometries
  - ➢ unavoidable temperature fluctuations
- Forward shifted method (`shifted`) [1]
- Emission-based Reciprocity Method (`ERM`) [2]
  - Rays also followed in a reverse direction: from detector to source

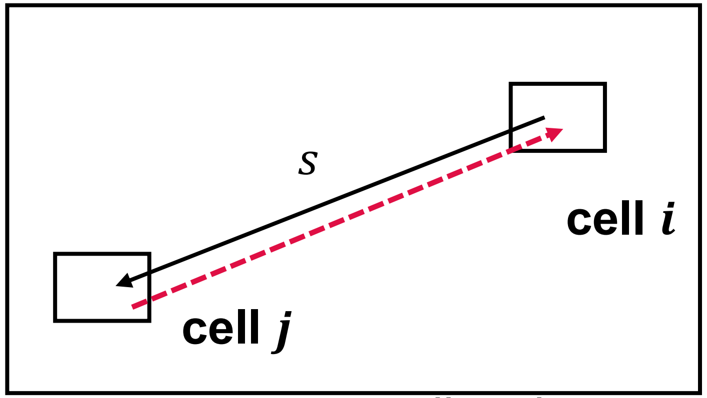
$$P_{i,j}^{exch} = \int_0^\infty \kappa_\eta I_b(T_i)\left(\frac{I_b(T_j)}{I_b(T_i)} - 1\right)\int_V \int_{4\pi} \tau(s)\, \alpha\, d\Omega dV d\eta$$

  - If $T_i == T_j$, then $P_{i,j}^{exch} = 0$. There is no radiative energy exchange between two volumes at same temperature, avoiding the unphysical fluctuation



MC algorithms, figures by X. Liu

⟶ forward direction



------➝ reverse direction

[1] L. Soucasse et al., “Monte Carlo methods for radiative transfer in quasi-isothermal participating media”, Journal of Quantitative Spectroscopy and Radiative Transfer 128, 2013
[2] L. Tessé et al., “Radiative transfer in real gases using reciprocal and forward Monte Carlo methods and a correlated-k approach”, IJHMT 5(13):2797-281, 2002

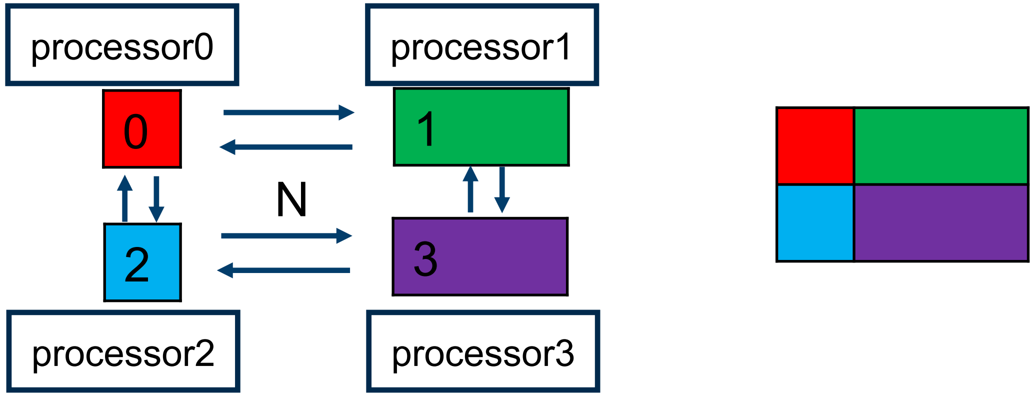
credits to X. Liu

MONTE CARLO SOLVER

JÜLICH Forschungszentrum

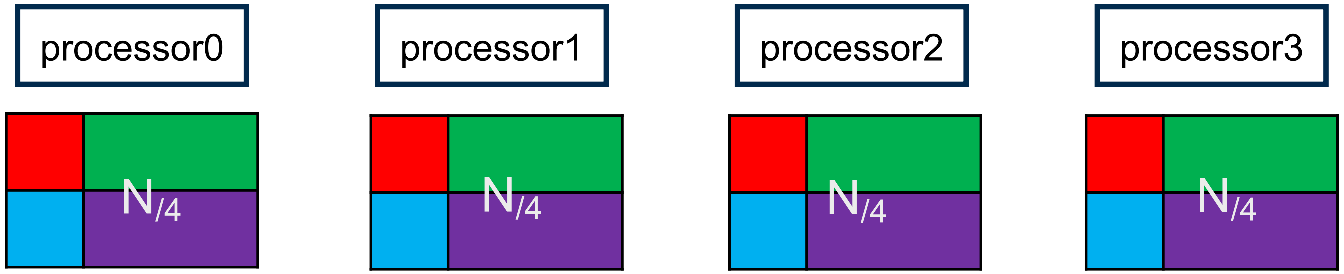
Monte Carlo Solver Efficiency Improvement: Efficient parallelization

- Domain decomposition for parallelization of CFD analysis, coupling via ‘processor patches`



Paralellization strategies for fvMCM, figure by X. Liu

- High communication effort, inefficient for radiation transport → distribute photon number over cores



- reconstruct global mesh
- distribute photon bundles
- reduce radiative source term
- update local CFD fields

➢ Efficiency increase about 40% w.r.t to domain decomposition, but higher memory requirement for global mesh.

credits to X. Liu

MONTE CARLO SOLVER

JÜLICH Forschungszentrum

Monte Carlo Solver Efficiency Improvement: Importance Sampling Method

- Biased sampling is one of variance reduction methods to accelerate Monte Carlo

$$\sigma = \frac{S}{\sqrt{N}}$$

  - Determine the “important” region / scenario and locally sample more photon bundles
  - Currently, importance sampling based on the temperature and x_{H2O} is implemented in fvMCM solver.
  - The important sampling technology generates more photon bundles in ‘hot, steam rich’ regions, while reducing the number of photons outside without losing accuracy.
- Radiation-CFD coupling outside PIMPLE loop: Update only every n time steps

➢ computation time in order of CFD

credits to X. Liu

MONTE CARLO SOLVER

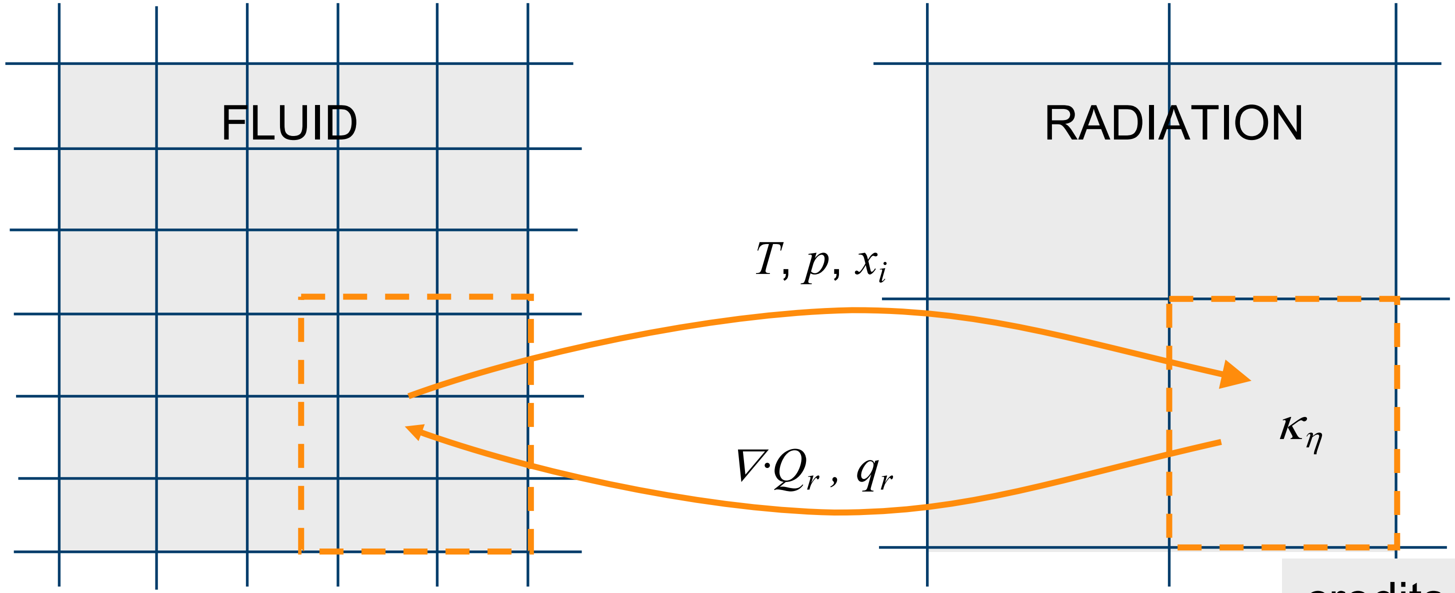
Monte Carlo Solver Efficiency Improvement: Mesh-to-Mesh projection

- Gradients of the radiation intensity are much less steep than those of velocity:
  - Radiation transport can be solved on a coarser mesh
  - Mapping of T, p, x_i from fluid to radiation mesh
  - Computing κ_η and solution of RTE on radiation mesh
  - Mapping of $\nabla \cdot Q_r$ and q_r from radiation to fluid mesh

➢ Reduction of the total photon count proportional to cell ratio

➢ Reduced efforts for photon tracking

➢ BPG ongoing

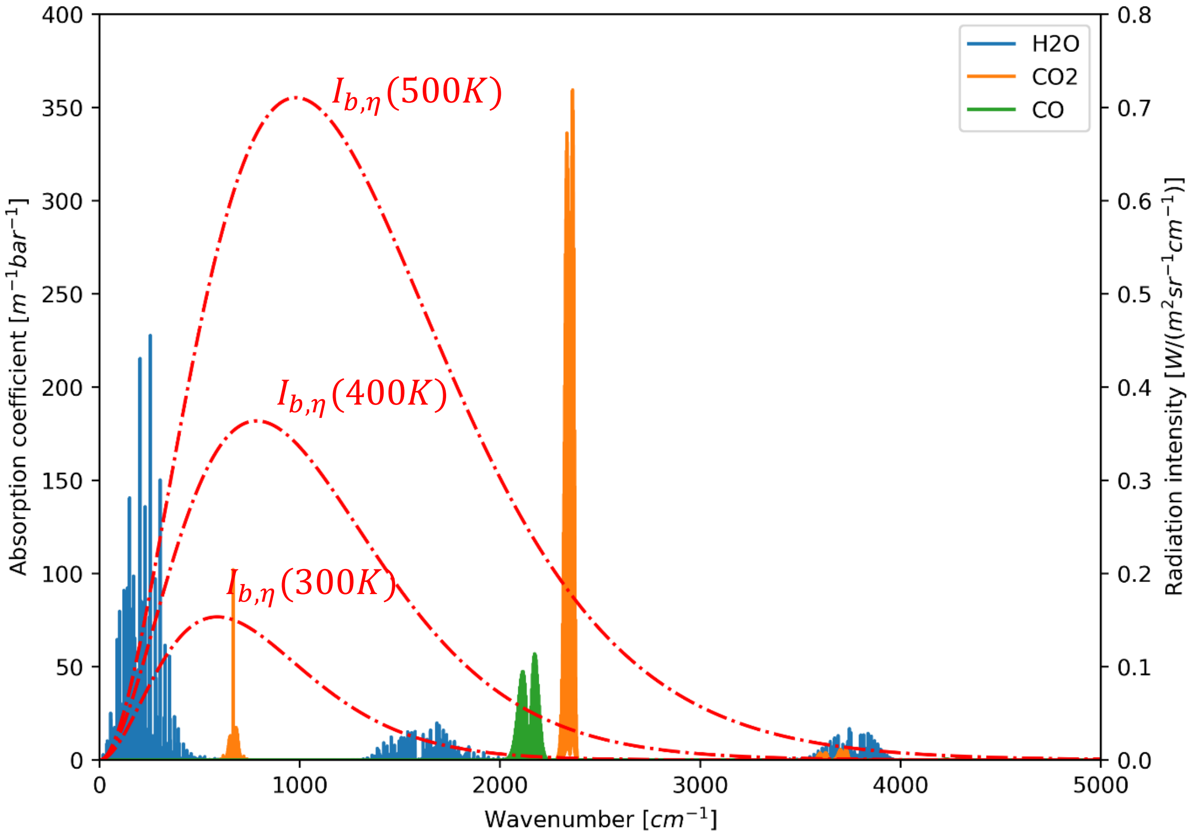


credits to X. Liu

SPECTRAL MODELING

Non-gray gas properties

- H_2O absorption spectrum is different from CO and CO_2
- The accuracy of the radiative source term depends on both prevailing spectral intensity and absorption spectrum of the gas mixture
- Nongray gas property is a function of $\eta, T, p_{H_2O}, p_{CO}$



Absorption coefficients vs. black body spectrum, figure by X. Liu

credits to X. Liu

SPECTRAL MODELING

JÜLICH Forschungszentrum

Overview

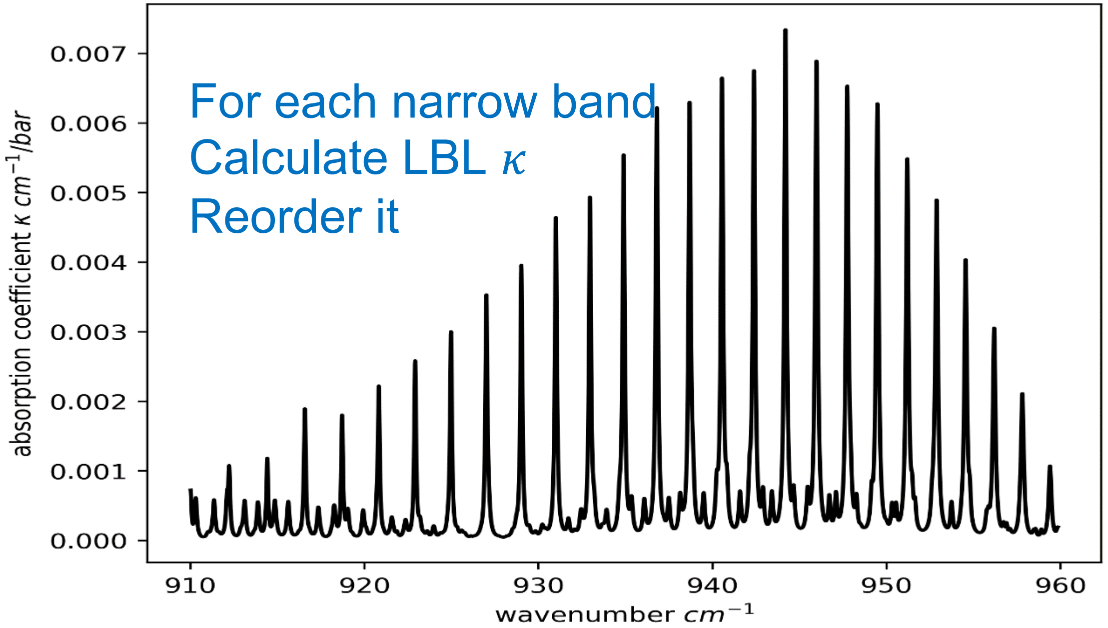
- Containment conditions during a severe accident
  - steam concentration (~5..80 vol.%) + CO, CO_2 (~0..10 vol.%)
  - gas temperature (30..250 °C)
  - large geometries (path length O ~ m)
  - Long transient with varying conditions (O ~ hours)
  - ➢ Different from combustion applications
  - ➢ Requirements:
    - Model applicable to full range
    - efficient

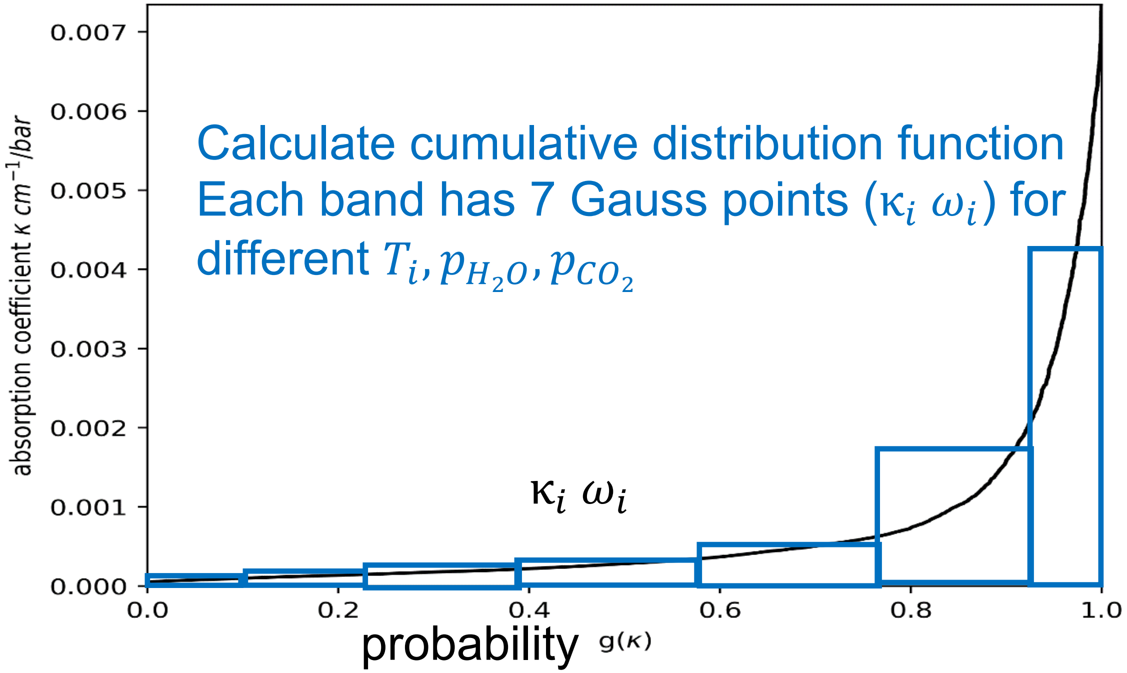
model	spectral lines	property
Line-by-Line (LBL)	~ 1 million	κ
Statistical Narrow Band correlated-k (SNBCK)	~ 200	κ
Statistical Narrow Band (SNB)	~ 200	τ
Exponential Wide Band model	~ 20	τ
Weighted-sum-of-grey-gases	~ 4	$\kappa i \cdot ai(T)$
Gray gas model	1	κ

credits to X. Liu

NONGRAY GAS PROPERTIES

Statistical narrow band correlated-k model (SNBCK)





$$\tau_{\Delta\eta} = \frac{1}{\Delta\eta}\int_{\Delta\eta} \tau(\kappa_\eta)\, d\eta \approx \sum_{i}^{nGauss} \omega_i\, \tau(\kappa_i)$$

$$I_{\Delta\eta} = \frac{1}{\Delta\eta}\int_{\Delta\eta} I(\kappa_\eta)\, d\eta \approx \sum_{i}^{nGauss} \omega_i\, I(\kappa_i)$$

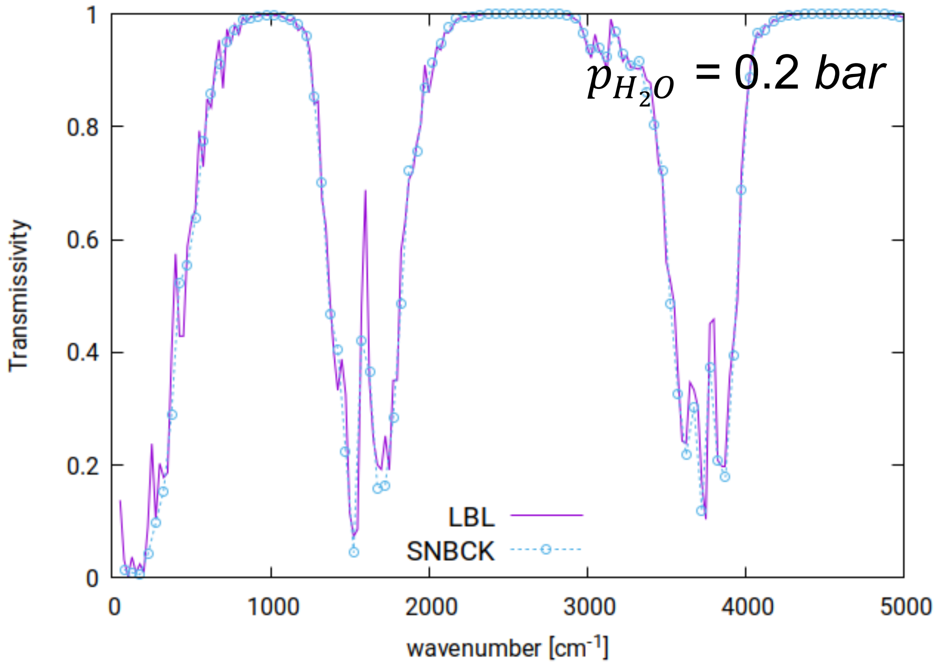
📖 Soufiani et al. "High temperature gas radiative property parameters of statistical narrow-band model for H_2O, CO_2 and CO, and correlated-K model for H_2O and CO_2" *IJHMT 40*(4), 987-991

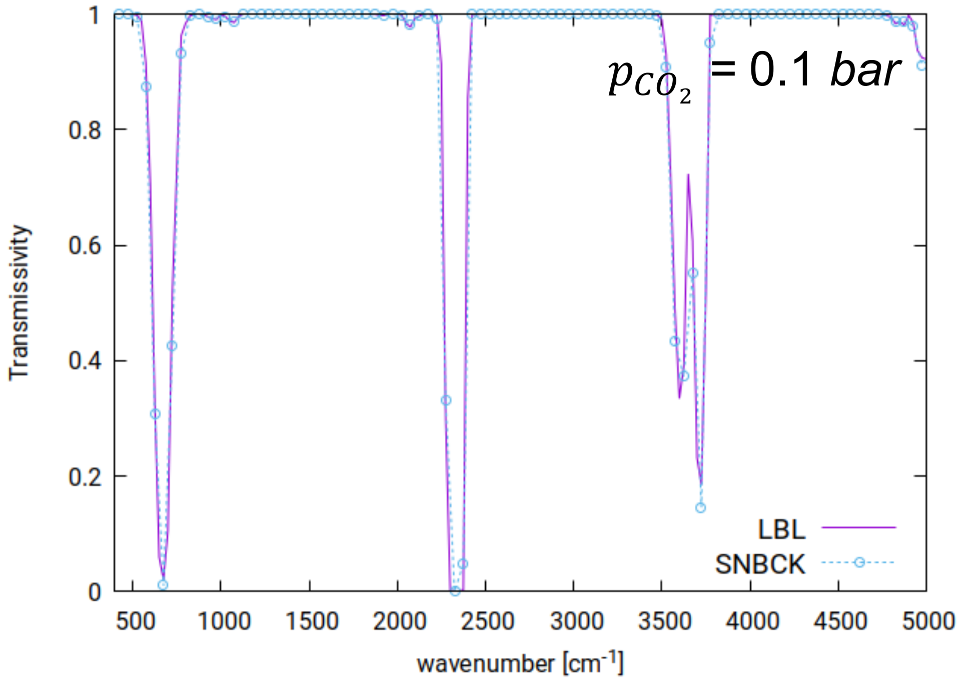
credits to X. Liu

NONGRAY GAS PROPERTIES

Verification agains LBL solutions

- Tailored SNBCK database for containment conditions





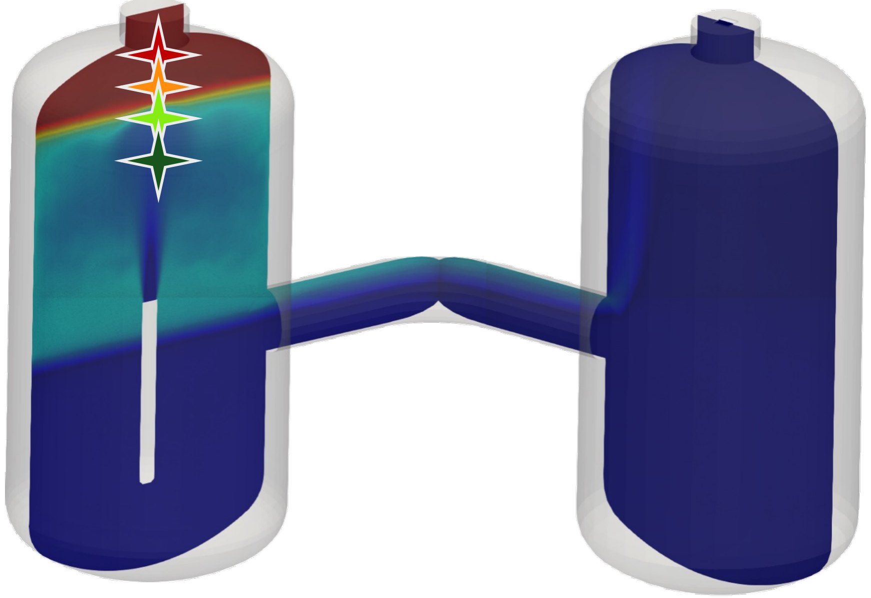
T = 400 *K*
p_{tot} = 1 *bar*
L = 1.0 *m*

credits to X. Liu

CONTAINMENTFOAM

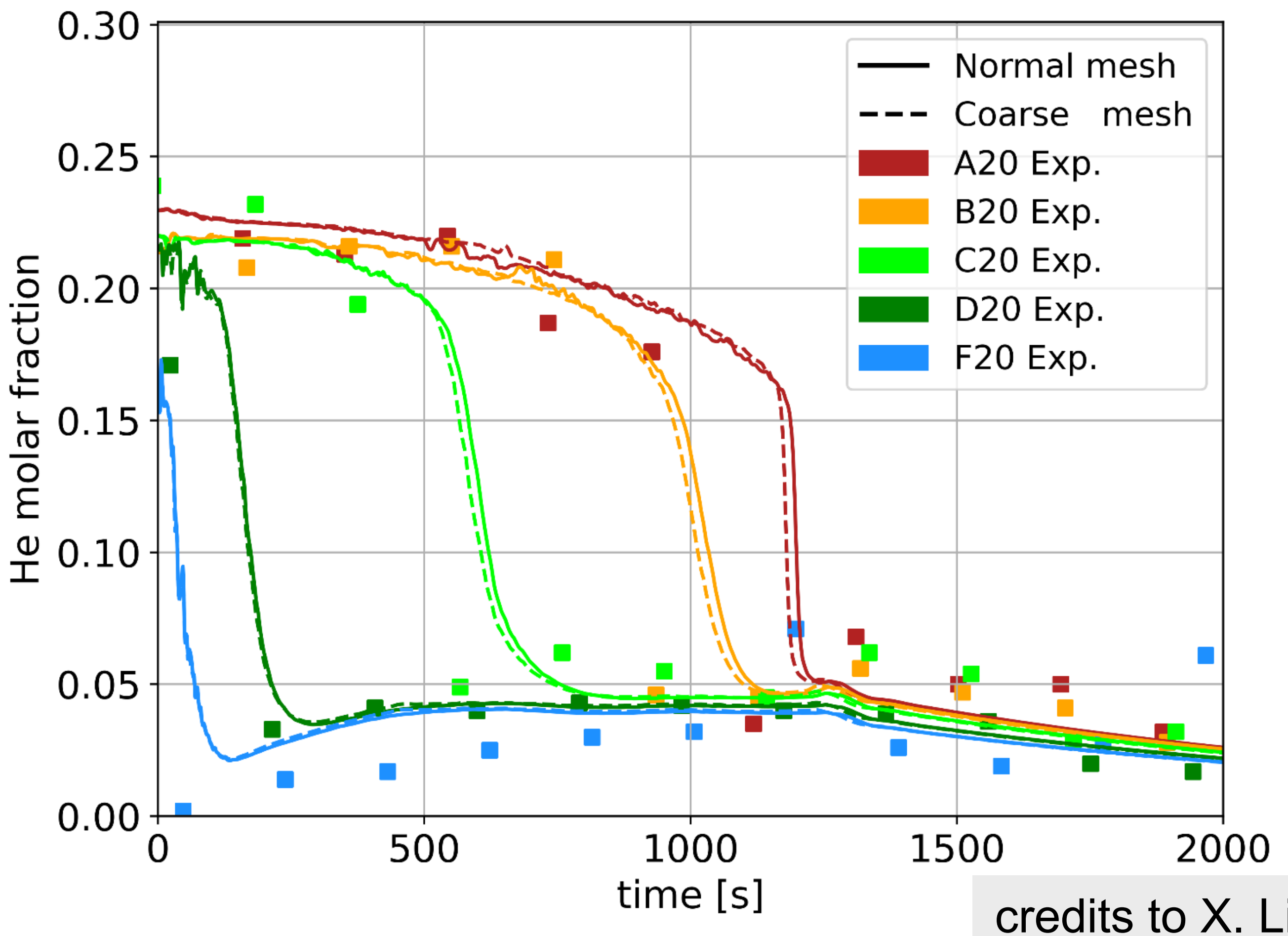
fvMCM-ERM Validation and Verification

- OECD/NEA SETH2 ST1_1_2
  - Radiation mesh 1/8th of CFD mesh



  - Radiation solver run time reduced from ~ 80% to 30% CFD runtime

➢ BPG needed on coarsening strategy



credits to X. Liu

GAS RADIATION MODELING

How to use it ?

- contant/radiationProperties

```
radiationModel              fvMCSNBCKH2OCO2;
fvMCSNBCKH2OCO2ParcelCoeffs
{
   minPhoton               40;
   maxPhoton               80;
   facePhoton              80;
   mode                    ERM;
   cutoff                  1e-4;
   nBatch                  1;
   globalMesh              true;
   conjugateHeatTransfer true;
   solverFreq              200;
}
absorptionEmissionModel  SNBCKH2OCO2AbsorptionEmission;
SNBCKH2OCO2AbsorptionEmissionCoeffs
{
 H2Ofilename  SNBCKH2O_300K_1100K_159bands.dat;
 CO2filename SBCKCO2_300K_1100K_159bands.dat;
}
```

- minPhoton: default 40, minimum for importance sampling
- maxPhoton: default 80, maximum for importance sampling
- facePhoton: default 80
- mode: MC algorithm: normal, shifted, ERM (default)
- cutoff: min photon energy
- nBatch: default 1, splits photons into batches to calculate stat. Error ‘MCrel‘
- globalMesh: default true, disable if memory constraints exist
- conjugateHeatTransfer: activate in case of multi region simulation
- solverFreq: number of flow iterations per radiation iteration (typically every 1s one update)
- absorptionEmissionModel / Coeffs: definition of the spectral model and database files

MODELING TECHNICAL SYSTEMS

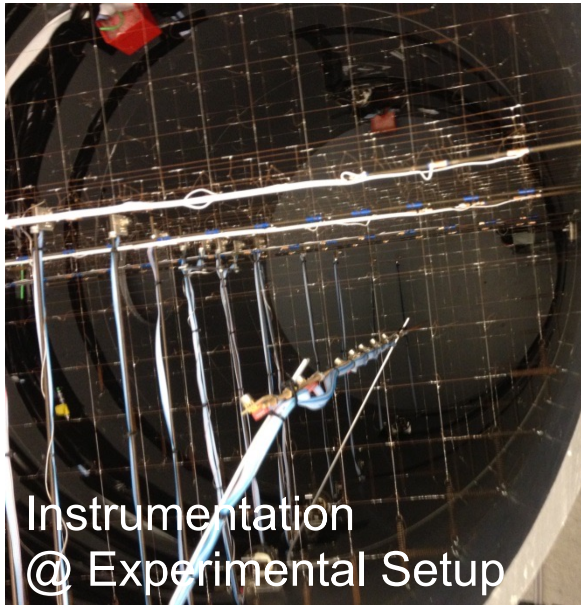
Introduction

- Major aspect of containent analysis is to assess efficiency of safety systems (in a severe accident typically only passive systems available)
  - Pressure relief flaps, blow-out panels, burst foils, doors
  - Passive auto-catalytic recombiners
  - Heat exchangers / unresolved structures (distributed heat sinks)
  - Sprinklers
  - Containment venting
  - Pressure suppression system
  - Emergency injection system
  - ..

POROUS MEDIA

Introduction

- While a CFD domain can be a large free volume, reality isn't !



- Resolving small structures (e.g., walking grids, filters, tube bundles) the mesh is often impossible in a technical-scale analysis.
- We must model their effects, e.g., flow resistance/pressure drop, thermal inertia and change in flow direction, production/dissipation of turbulence.

POROUS MEDIA

Concept

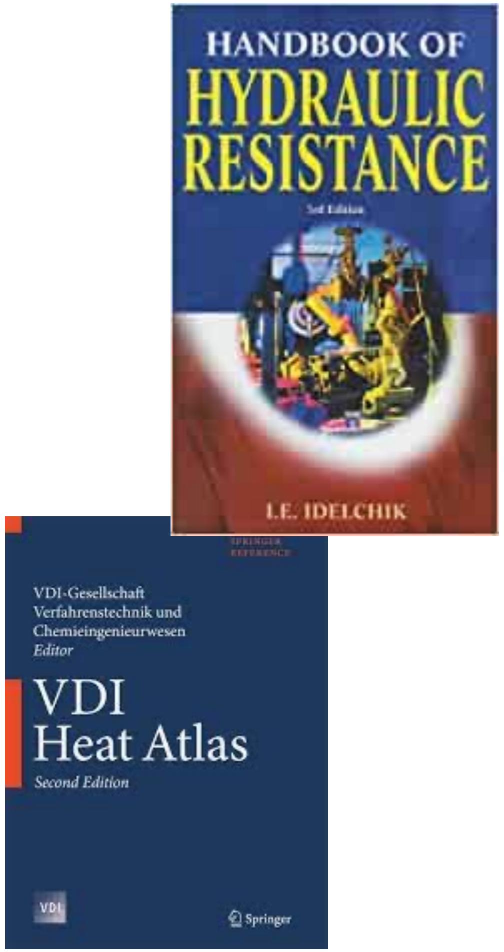
- Darcy-Forchheimer model adds a new sink to momentum equation:

$$\nabla p = \left(\underbrace{\mu \vec{D}}_{\text{Darcy}} + \underbrace{\frac{1}{2} \rho \vec{F} \vec{U}}_{\text{Forchheimer}} \right) \vec{U}$$

  - Darcy (linear) and Forchheimer (quadratic) loss coefficients can be specified in streamwise and transversal directions

- How to obtain coefficients?
  - Text books:
    - Standard geometries

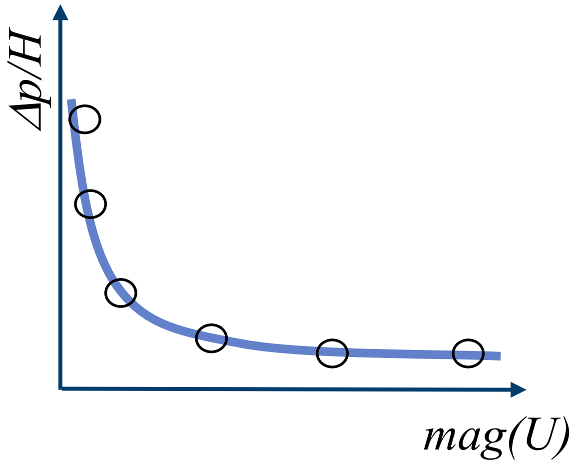
$$\Delta p = \left(\lambda \frac{L}{d_H} + \xi \right) \frac{1}{2} \rho U^2$$



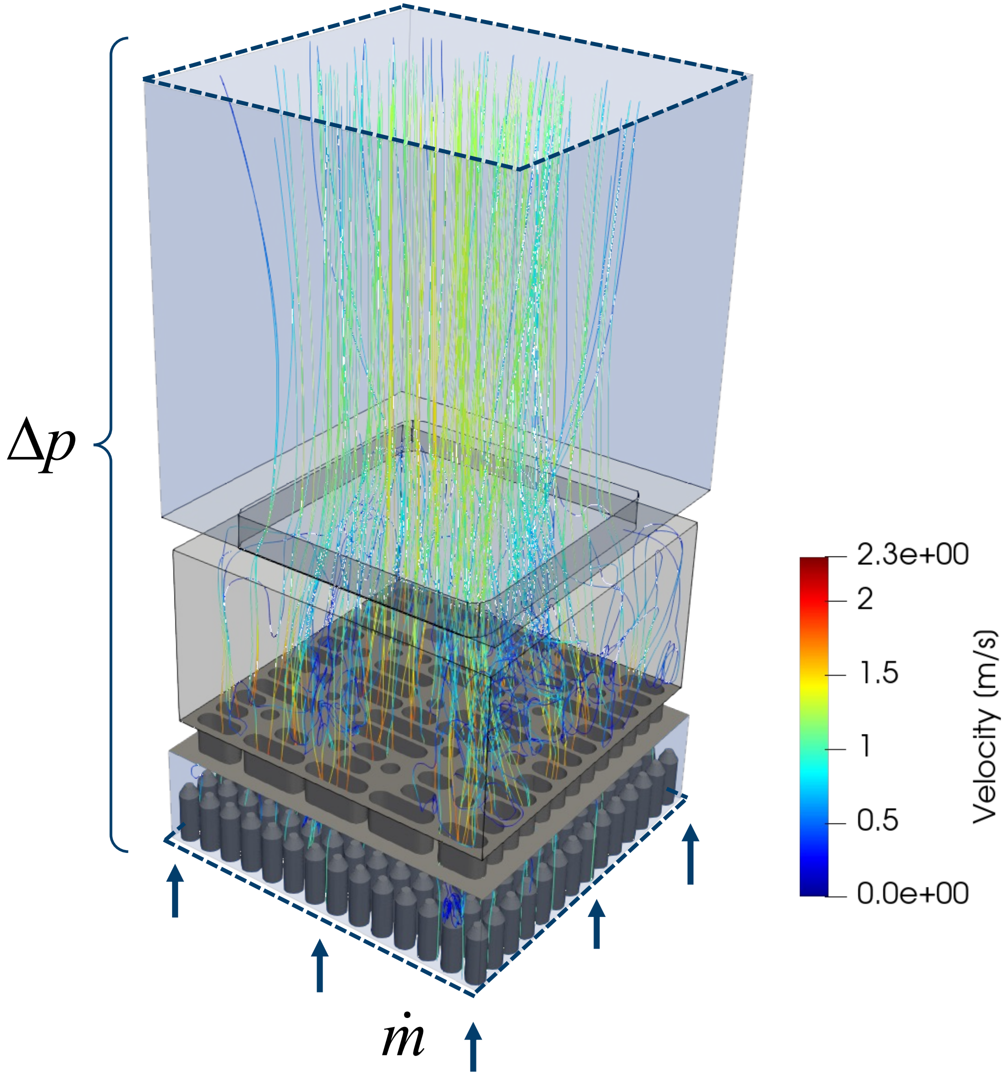
POROUS MEDIA

Concept

- How to obtain coefficients?
  - detailed CFD analysis
    - non-standard geometries
    - Determine polynomial fit for $\Delta p(U)$



$$\Delta p / H = \left(K_{loss}\right)\frac{1}{2}\rho U^2$$



POROUS MEDIA

How to use it ?

- constant/fvModels

```
type              explicitPorositySource;
explicitPorositySourceCoeffs {
  selectionMode   cellZone;
  cellZone        GRIDZONE;
  type            DarcyForchheimer;
  DarcyForchheimerCoeffs        {
     d   d [0 -2 0 0 0 0 0] (0 0 0);
     f   f [0 -1 0 0 0 0 0] (1000 15 1000);
     coordinateSystem
     {
        type    cartesian;
        origin  (0 0 0);
        coordinateRotation
        {
          type    axesRotation;
          e1  (1 0 0);
          e2  (0 0.96456 -0.26387);
}}}}
```

all, cellSet, cellZone, points

definition of porous region

Darcy coefficient, mostly (0 0 0)

Forchheimer coefficient, isentropic or directional

coordinate system for d and f vectors;
e1 and e2 are unit vectors; e3 = e1 x e2

POROUS MEDIA

Heat transfer – porous CHT

- Preserving heat capacity of unresolved structures in a system-scale model:
  - multiRegion approach (1 mesh for fluid region, 1 mesh for porous solid) coupled by `fvModels` definition in each region

constant/FLUID/fvModels

```
type                constantHeatTransfer;
nbrRegionName       GRID;
interpolationMethod cellVolumeWeight;
nbrModel            porousCHT;
fields              (h);
semiImplicit        false;
```

- type: model to be applied (variableHeatTransfer or tabulatedHeatTransfer)
- nbrRegionName: coupled region name
- interpolationMethod: mapping method
- nbrModel: name of fvModels object on solid side
- fields: field to be mapped

constant/GRID/fvModels

```
type                constantHeatTransfer;
nbrRegionName       FLUID;
interpolationMethod cellVolumeWeight;
nbrModel            porousCHT;
fields              (h);
semiImplicit        false;
```

variableHeatTransfer: $Nu = a \cdot \mathrm{Re}^b \cdot \mathrm{Pr}^c$

https://cpp.openfoam.org/v9/classFoam_1_1fv_1_1interRegionHeatTransfer.html#details

POROUS MEDIA

Scalar sources

- Damping turbulence: While passing through the narrow channels, large eddies break up into small ones, which are quickly dissipated → damping of turbulence

constant/FLUID/fvConstraint

```
type            fixedValueConstraint;
selectionMode   cellZone;
cellZone        GRIDZONE;
fieldValues     {
   k          0.05;
   omega      300;
}}
```

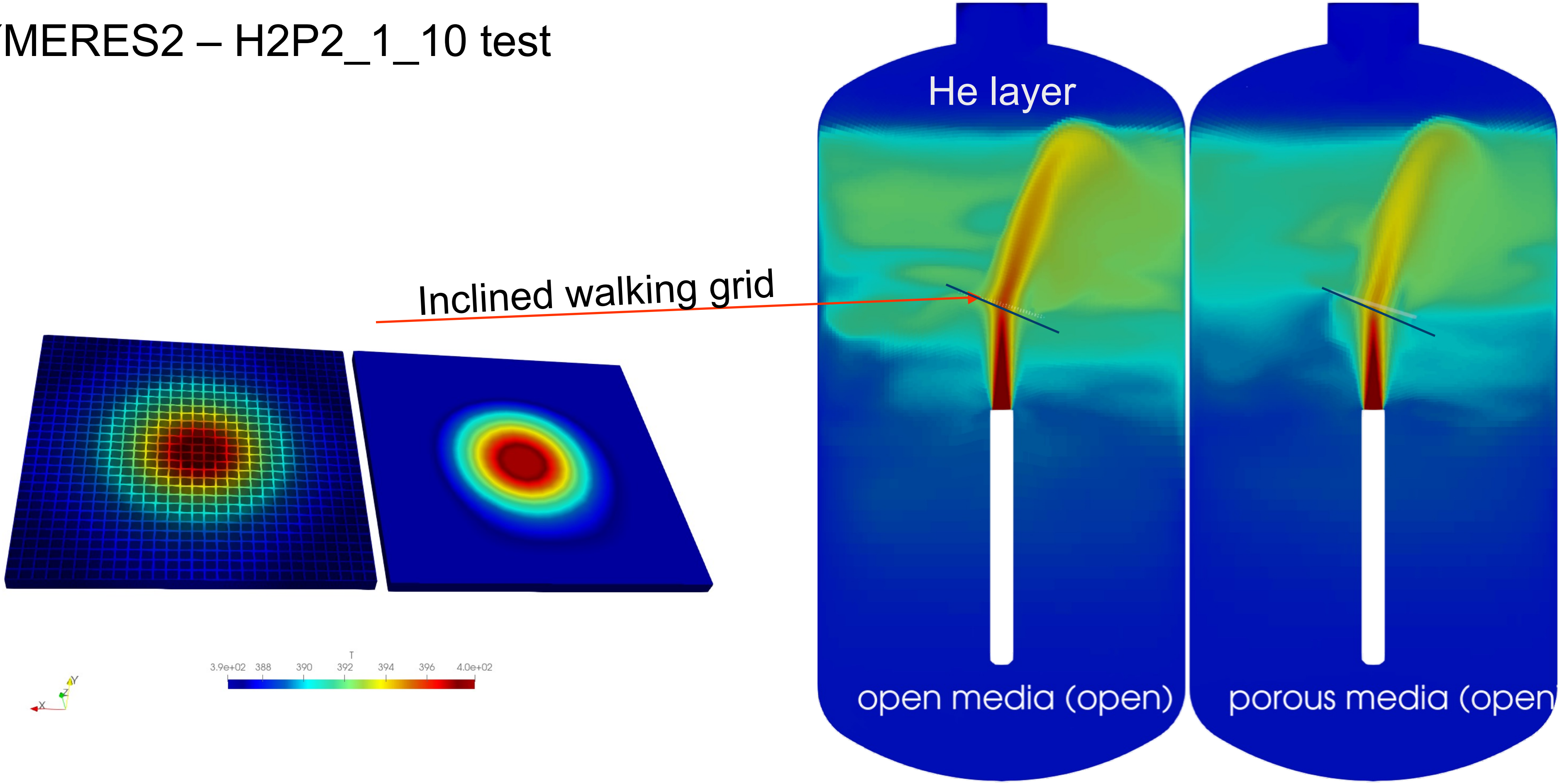
- `type`: model to be applied (e.g. limitPressure, limitTemperature)
- `cellZone`: definition of porous region
- `fieldValues`: volScalarFields to be overwritten by value

https://cpp.openfoam.org/v9/classFoam_1_1fvConstraint.html

POROUS MEDIA

Application – walking grid

- OECD/NEA HYMERES2 – H2P2_1_10 test



POROUS MEDIA

Heat sources

- Modeling a heat exchanger:
  - Description of a (transient) heat source

constant/FLUID/fvModels

```
type                 heatSource;      <- fvModel to be applied
selectionMode        cellSet;
cellSet              HEATER;          <- definition of porous region
Q                    1e6;             <- Scalar source or function1 type (e.g. table, csvFile)
```

https://cpp.openfoam.org/v9/classFoam_1_1fvModel.html

POROUS MEDIA

Heat sources

- Modeling a heat exchanger:
  - Simple built-in heat exchanger model $$\dot{Q}_{tot} = e(\phi_{in}, \dot{m}_2)(T_2 - T_1)\phi_{in} c_p$$

constant/FLUID/fvModels

```
type   effectivenessHeatExchangerSource;
selectionMode             cellZone;
cellZone                  htx;
secondaryMassFlowRate     1.0;
secondaryInletT           336;
primaryInletT             293;

faceZone               facesZoneInletOriented;
effectiveness             <function2>;
```

- type: fvModel to be applied
- cellZone: definition of porous region
- faceZone: used to integrate the net mass flow rate ϕ_{in} into the heat exchanger
- effectiveness: described in terms of the primary and secondary mass flow rates

  - Distribution to cells based on local velocity and temperatures

https://cpp.openfoam.org/v9/classFoam_1_1fv_1_1effectivenessHeatExchangerSource.html#details

POROUS MEDIA

JÜLICH Forschungszentrum

Mass (continuity) sources

- When modeling small distributed mass sources/sinks, one has to take care of transported quantities

constant/FLUID/fvModels

```
type            massSource;
selectionMode   cellZone;
cellZone        INJECTIONRING;
fields          (rho U H2O h k omega);
massFlowRate    table
   ((0.0    0.24)
    (5.0    0.48)
    (10.0 -0.10));
mode            internal;
fieldValues {
    U           constant (0 2 0);
    ..}
```

definition of release location

definition of all solution fields (except pressure) in the present case

definition of mass flow rate constant or function1

Internal: uses local field value (sources and sinks), external uses specified fieldValues (only sources)

values should be provided for all solved for fields

https://cpp.openfoam.org/v9/classFoam_1_1fv_1_1massSource.html

MODELING TECHNICAL SYSTEMS

Pressure dependent flow path

- BurstDisc model:
  - Opens as soon as a differential pressure / net force between both sides is exceeded
  - Basic functionality in OpenFOAM:
    blends between baffle / cyclic patch pair
  - Pre-processing:
    - Create ‚baffle' + ‚cyclic' patch pair using the same faces
      - create face set: topoSet (from exisiting patches, surfaces, primitive volumes..)
      - remove existing baffles: mergeBaffles
      - create patch pair: createBaffles

constant/polyMesh/boundary

```
BURSTDISC2_side1    {
   type       cyclic;
   inGroups   list<word>  1(cyclic);
   nFaces     25;
   startFace  4310;
   matchTolerance   0.0001;
   neighbourPatch   BURSTDISC2_side2;
   transformType    none;     }
BURSTDISC2_side2    {
   type       cyclic;
   inGroups   list<word>  1(cyclic);
   nFaces     25;
   startFace  4335;
   matchTolerance   0.0001;
   neighbourPatch   BURSTDISC2_side1;
   transformType    none;     }
BURSTDISC2          {
   type       wall;
   inGroups   List<word>  1(wall);
   nFaces     50;
   startFace  4360;  }
```

MODELING TECHNICAL SYSTEMS

Pressure dependent flow path

- BurstDisc model:
  - Pre-processing:
    - Create ‚baffle' + ‚cyclic' patch pair using the same faces
    - Set-up boundary conditions:
      - 0/U: Holds activation parameters
      - 0/others: cyclic / baffle wall definition
  - Solving:
    - system/systemEvents → estimated opening time

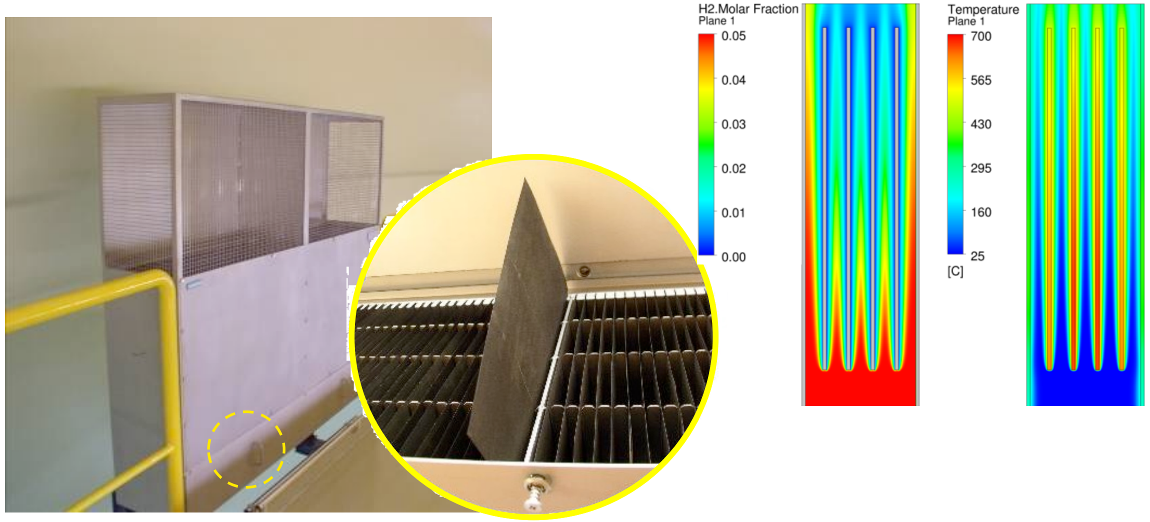
0/U

```
BURSTDISC2_side1    {
   type    cyclic;
}
BURSTDISC2_side2    {
 type       cyclic;
}
BURSTDISC2          {
   type          burstDisc;
   cyclicPatch   BURSTDISC2_side1;
   orientation   1;
   openingTime   3;
   maxOpenFractionDelta   0.1;
   openFraction 0;
   forceBased   false;
   minThresholdValue  1000;
   value uniform (0 0 0);
```

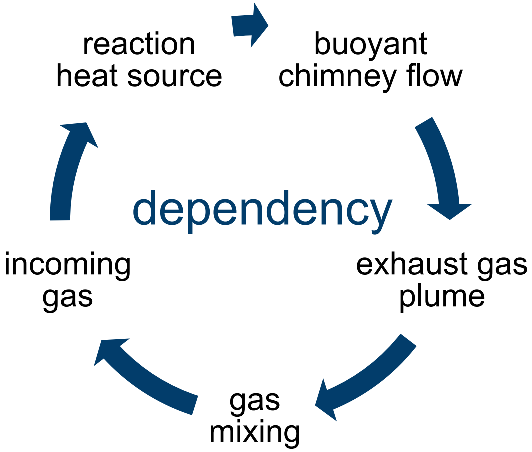
MODELING TECHNICAL SYSTEMS

Example - Passive Auto-Catalytic Recombiners

- Flameless exothermal conversion of
  - $H_2 + \frac{1}{2} O_2 \rightarrow H_2O + 242\ kJ/mol$
  - $CO + \frac{1}{2} O_2 \rightarrow CO_2 + 282\ kJ/mol$
  - Passive, buoyancy driven flow
- Typically ~ 60 PARs are installed in a large dry PWR
- Importance of CFD for PAR design:
  - Detailed design (catalyst, housing)
  - Placement inside a compartment (hot exhaust plume, stagnant zones)
- Scales:
  - Catalyst surface μm – catalyst spacing cm – PAR size m
  - Can hardly be resolved in system scale CFD applications



PAR concept and passive operation, own figures



MODELING TECHNICAL SYSTEMS

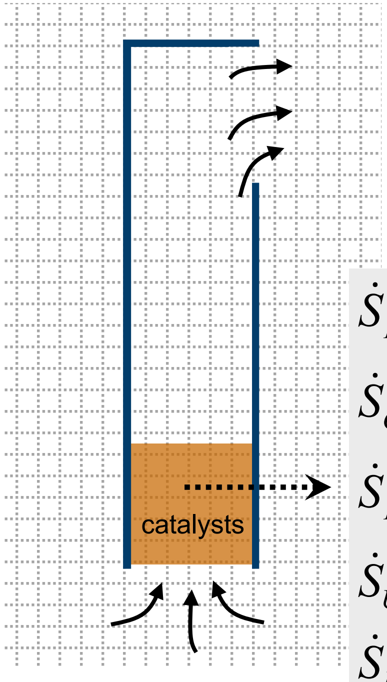
JÜLICH Forschungszentrum

Passive Auto-Catalytic Recombiners – Porous media

- Option 1: Porous / homogeneous model
  - Momentum loss: porous media approach
  - Reaction heat release: manufacturers correlations, e.g.

$$\dot{m}_{H_2} = \min\left[\nu_{H_2}, \frac{2.0\cdot(\nu_{O_2}\cdot\nu_{H_2})}{(\nu_{H_2}+\nu_{CO})}, 8.0\cdot\frac{\nu_{H_2}\cdot(\nu_{H_2}+1.75\cdot\nu_{CO})}{(\nu_{H_2}+\nu_{CO})^2}\right]\cdot(k_1\cdot p + k_2)$$
$$\cdot\tanh(\nu_{H_2}+\nu_{CO}-\nu_{min})\cdot c_1$$

📖 framatome „Correlations for Hydrogen and Carbon Monoxide Recombination by Framatome Passive Autocatalytic Recombiners", Technical Report D02-ARV-01-143-222, 2019



$$\dot{S}'''_{H2,m} = -\dot{m}_{H2}\cdot\frac{V_{cell}}{V_{cat}}$$

$$\dot{S}'''_{O2,m} = -\dot{m}_{H2}\cdot\frac{M_{H2}}{M_{O2}}\cdot\frac{V_{cell}}{V_{cat}}$$

$$\dot{S}'''_{H2O,m} = \dot{m}_{H2}\cdot\frac{M_{H2}}{M_{H2O}}\cdot\frac{V_{cell}}{V_{cat}}$$

$$\dot{S}'''_{U} = -\zeta\cdot\frac{1}{2}\rho U^2$$

$$\dot{S}'''_{h} = \dot{m}_{H2}\cdot\Delta h_R$$

  - Source and sink terms for change in mixture composition
  - Model and user parameters e.g. k_1, k_2 or min. reactants concentration v_{min}

➢ Straight forward implementation, but limited generality to a vast range of operating conditions or phenomena e.g. poisoning, ignition etc.

MODELING TECHNICAL SYSTEMS

Passive Auto-Catalytic Recombiners

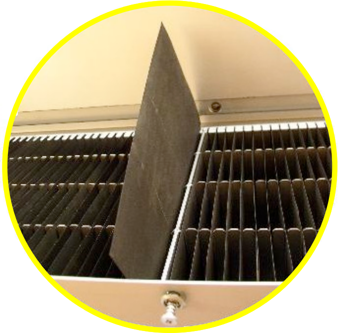
- Option 2: Code coupling
  - REKODIREKT code for a single PAR of Framatome, AECL (and NIS) type
  - Sub models:
    - Poisoning
    - Start-up
    - Ignition
    - Counter-current flow

PAR	Phenomena	REKO-DIREKT

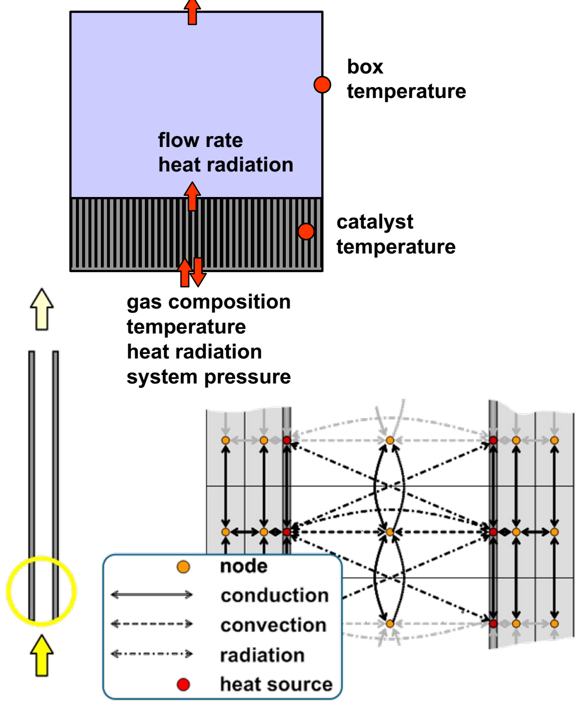
PAR housing / chimney

- Buoyancy driven flow
- Thermal inertia and heat losses to the environment

Catalyst section



- Reaction kinetics, incl. O_2 starvation, humidity, parallel CO recombination by transport approach
- Heat distribution, thermal inertia



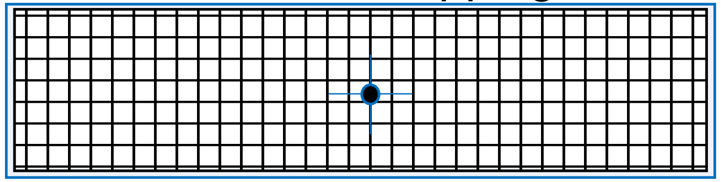
📖 Reinecke et al, "Validation and Application of the REKO-DIREKT Code for the Simulation of Passive Autocatalytic Recombiner Operational Behavior", Nuclear Technology 196,2,2016
📖 M. Klauck et al., "Effect of PAR deactivation by carbon monoxide in the late phase of a severe accident" Annals of Nuclear Energy 151 (2021) 107887

MODELING TECHNICAL SYSTEMS

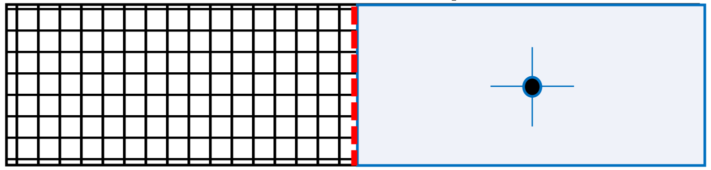
Passive Auto-Catalytic Recombiners

- Option 2: Code coupling
  - Spatial coupling:

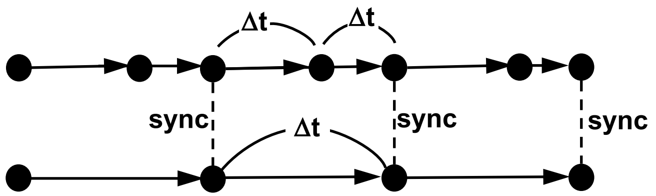
‚domain overlapping‘



‚domain decomposition‘



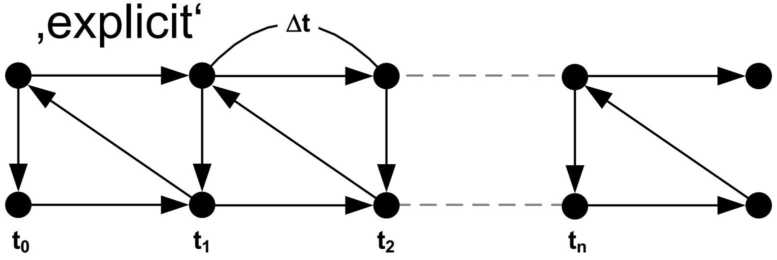
  - Transient coupling:
    - Subcycling/ Synchronization:



📖 Long et al. *Review of researches on coupled system and CFD codes*, Nuclear Engineering and Technology 53 (2021) 2775-2787

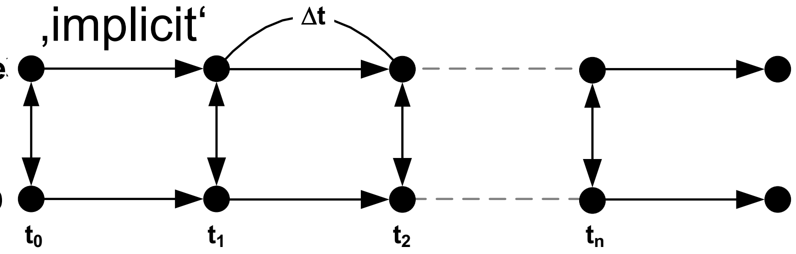
    - Coupling scheme:

‚explicit‘



RD-CFX: Explicit coupling scheme

‚implicit‘

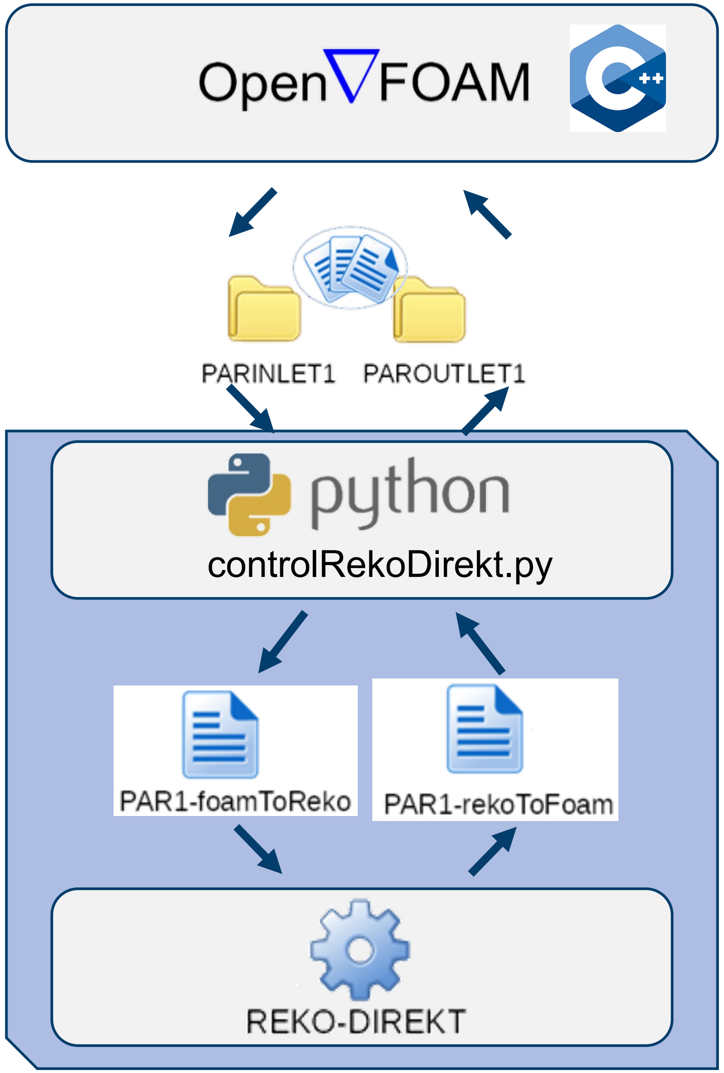


➢ Approach depends on physics, their individual time scales and possible constraints of the external code

MODELING TECHNICAL SYSTEMS

Example – containmentFOAM –REKODIREKT Coupling

- Option 2: Code coupling
  - Data logistics
    - Initialization of RD
    - Intermediate RD data storage
    - Convert data between OF (fields) and RD (scalars)
    - Organize data for arbitrary PAR types and numbers
    - Log-files / output
    - Backup & Restart

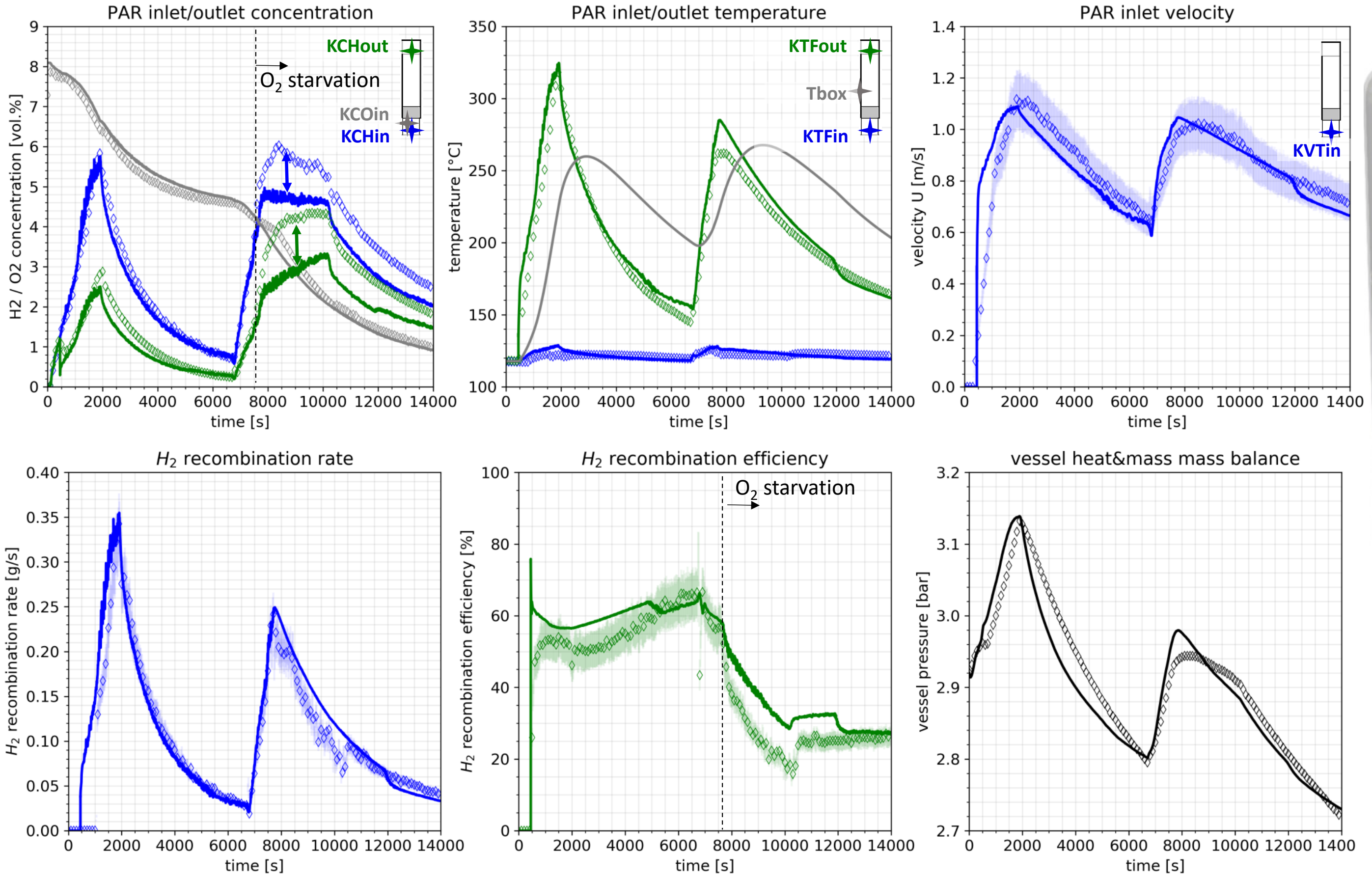


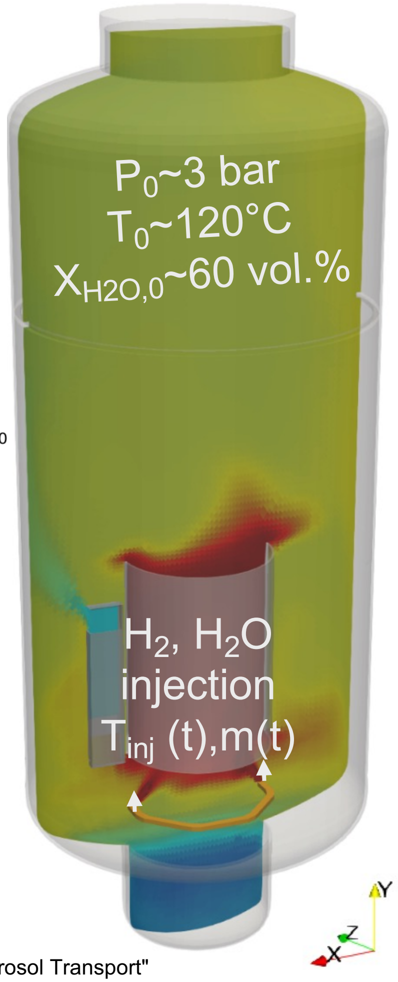
MODELING TECHNICAL SYSTEMS

Passive Auto-Catalytic Recombiners

- Model validation:
  - OECD/NEA THAI HR12:
    - Transient O_2 starvation
    - Wall condensation
    - Thermal stratification
    - Gas radiation

➢ Mechanistic approach reveals predictive capabilities for relevant conditions





Kelm, S. et al. "The Tailored CFD Package 'containmentFOAM' for Analysis of Containment Atmosphere Mixing, H_2/CO Mitigation and Aerosol Transport" *Fluids* (2021) 6, no. 3: 100. https://doi.org/10.3390/fluids6030100

MODELING TECHNICAL SYSTEMS

- How to use it

system/controlDict

```
type                      externalCoupled;
log                       false;
commsDir                  "comms";
initByExternal            no;
calcFrequency             1;
stateEnd                  remove;
regions {
    "region0" {
          PARINLET1 {
             readFields      (U);
             writeFields     (T O2 N2 H2O CO2 H2 CO p fog);
                    }
          PAROUTLET1 {
             readFields      (T U O2 N2 H2O CO2 H2 CO);
             writeFields     ();
}}}
```

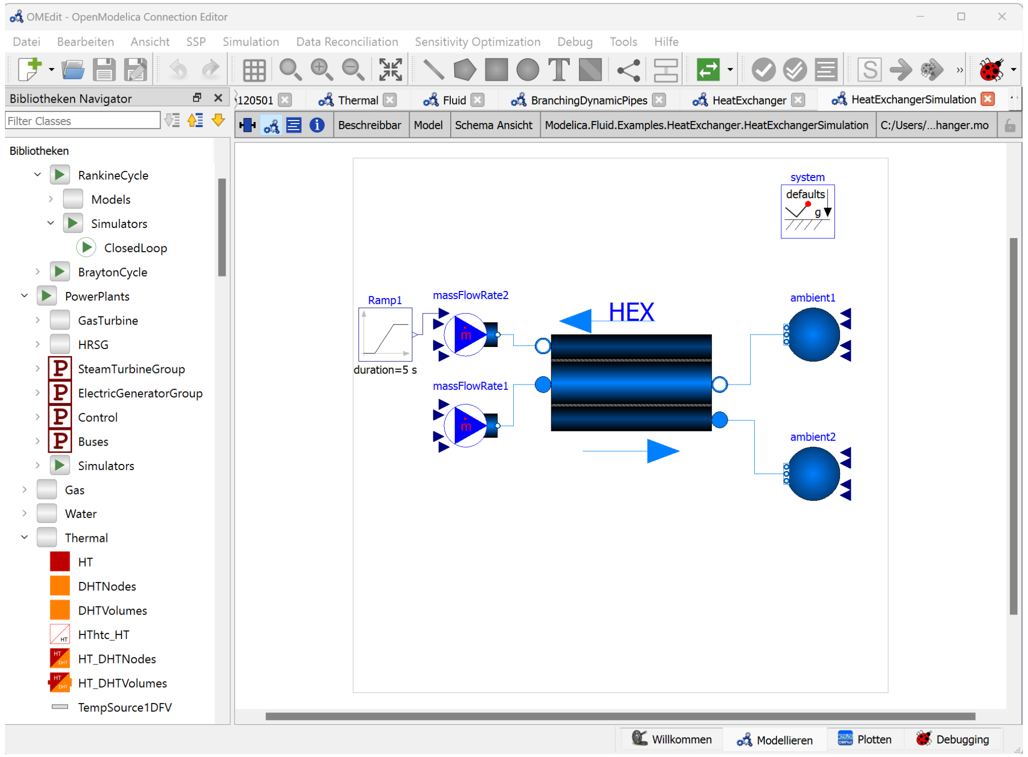
- commsDir: location of I/O exchange with ext. program
- calcFrequency: number of time steps per ext. program call
- "region0": name of region
- PARINLET1: name of coupling interface1
  - readFields: list of fields to read from ext. program
  - writeFields: list of fields to write from OpenFOAM
- PAROUTLET1: name of coupling interface2
  - readFields: list of fields to read from ext. program
  - writeFields: list of fields to write from OpenFOAM

- BC to update must be of specific type (`fixedValue, externalCoupledflowRateInletVelocity`)

MODELING TECHNICAL SYSTEMS

System modeling

- Coupling containment∇FOAM with OpenModelica
  - Modelica:
    - A modelling language designed for the study of engineering system dynamics
    - equation-based, modelling (DAE systems) in terms of physical/engineering principles (mass, energy and momentum balance + constitutive equation + constraints)
    - enables packaging and exporting Modelica system models as an executable simulator (Functional Mockup Units 'FMU') in accordance with the Functional Mock-up Interface 2.0 (FMI2) standard



https://openmodelica.org/

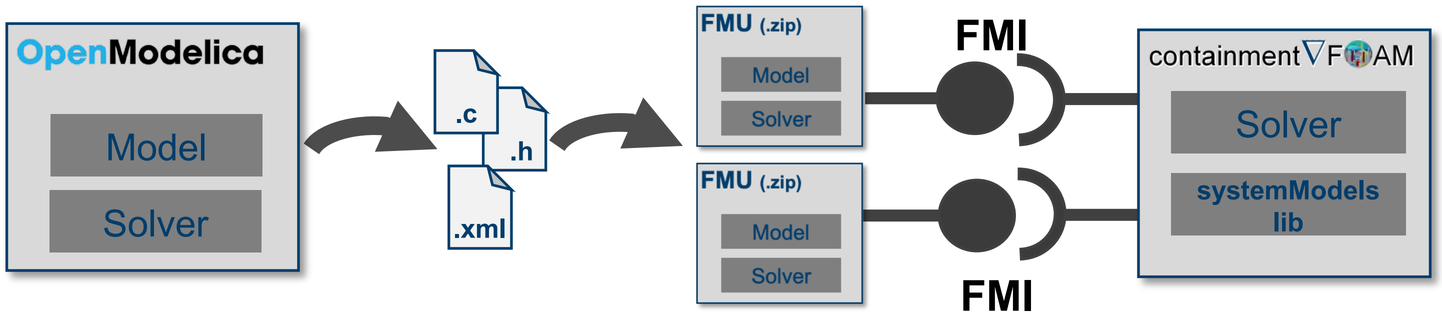
📖 P. Fritzson et al., "The OpenModelica Integrated Environment for Modeling, Simulation, and Model-Based Development," Modeling, Identification and Control: A Norwegian Research Bulletin, vol. 41, no. 4, pp. 241–295, 2020.

credits to K. Sturm

MODELING TECHNICAL SYSTEMS

System modeling

- Coupling containment∇FOAM with OpenModelica
  - Packaging FMU's for co-simulation via FMI (https://github.com/modelon-community/fmi-library)



  - generally, any program can be packaged into FMU's and provided for co-simulation (e.g., REKODIREKT)
- `systemModels` library:
  - C++ - implementation of FMU4FOAM functionality (https://pypi.org/project/FMU4FOAM) in containment∇FOAM
  - Explicit and semi-implicit coupling schemes incl. sub cycling of FMU
  - Restarts

📖 https://fmi-standard.org/
https://www.samares-engineering.com/en/2021/01/21/part-9-co-simulation-of-sysml-and-other-models-through-fmi/

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MODELING TECHNICAL SYSTEMS

System modeling

- Coupling containment∇FOAM with OpenModelica
  - Example: (simplified) Pressure Suppression System

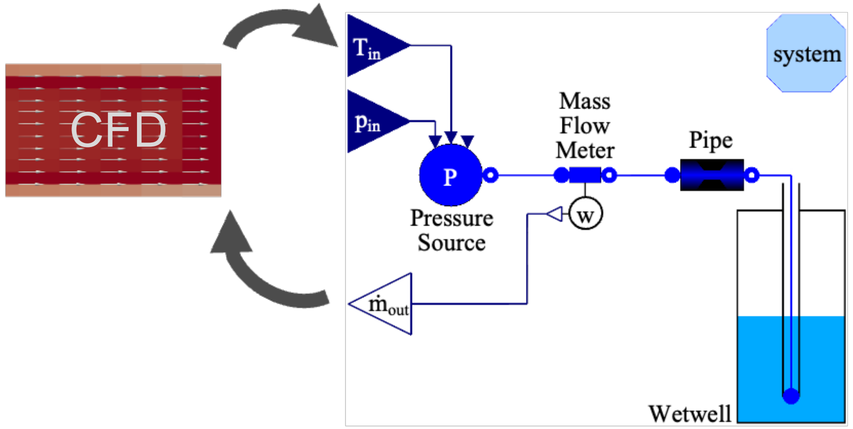
K. Sturm, *Development of a coupling scheme for Modelica and OpenFOAM to simulate the pressure suppression system of a SMR*, RWTH Aachen Aug. 2023

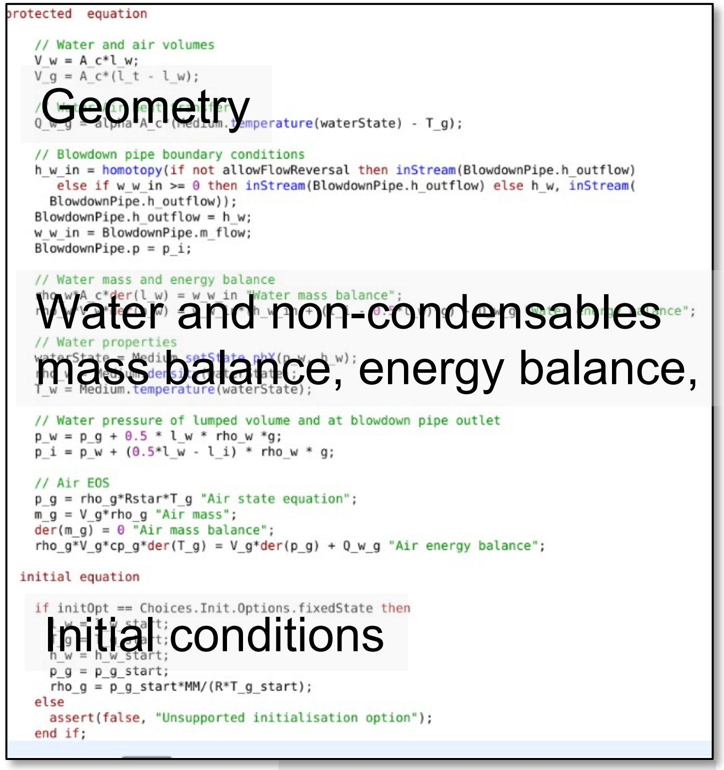
```
coupling     true;
scheme       explicit; // explicit, implicit
algorithm    none; // none, Aitken, Quasi-Newton

FMU {
    pss0 {
        name     PSS;
        path     "$FOAM_USER_LIBBIN/FMUs/PressureSuppression";
        log (
            p_in
            T_in
            w_out
            wetWell1.p_i
            wetWell1.T_w   );
}}

boundary {
    OUT {
        pressure {
            projection  maxValue;
            direction   output;
            extVar      p_in;
            fmu         pss0;
..
        }

        massflow {
            projection  integral;
            direction   input;
            extVar      w_out;
            fmu         pss0;
        }
    }
}
```





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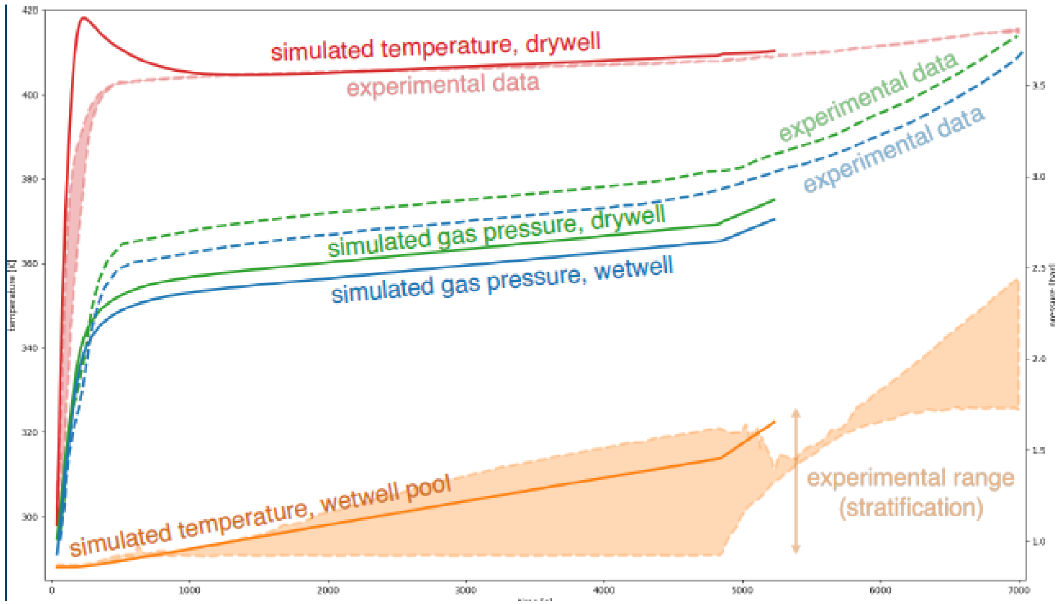
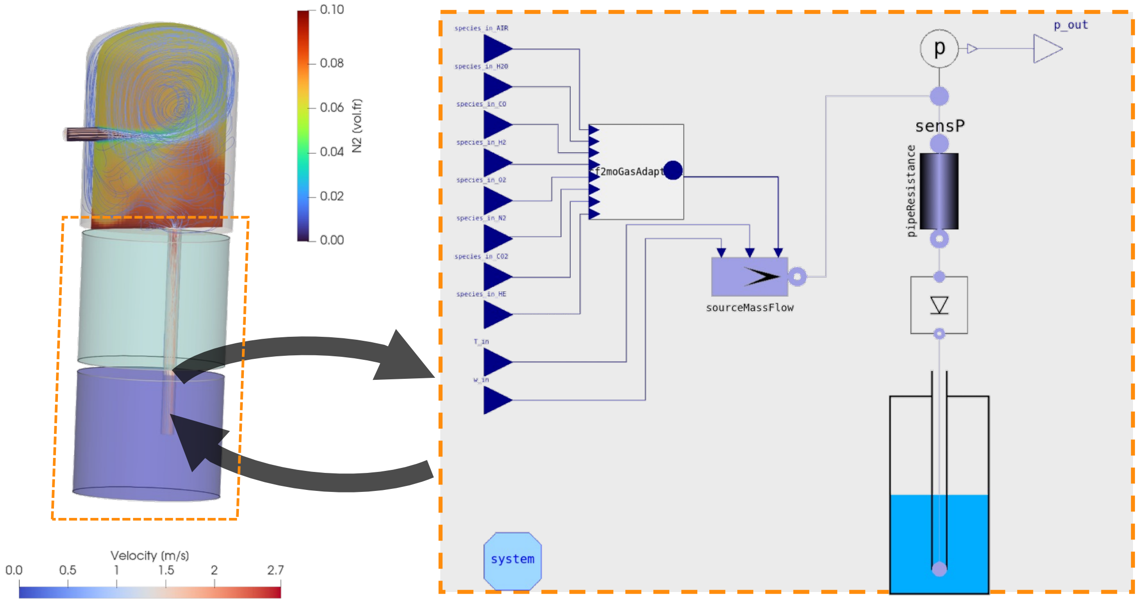
PERSPECTIVES

SMR Applications - System modeling

- Coupling containment∇FOAM with OpenModelica
  - Example: PPOOLEX mix05

📖 J. Laine, M. Puustinen, A. Räsänen, *PPOOLEX Experiments on the Dynamics of Free Water Surface in the Blowdown Pipe, Research report, LUT Lappeenranta, Feb. 2013*





📖 K. Sturm, *Development of a coupling scheme for Modelica and OpenFOAM to simulate the pressure suppression system of a SMR,* RWTH Aachen Aug. 2023

credits to K. Sturm

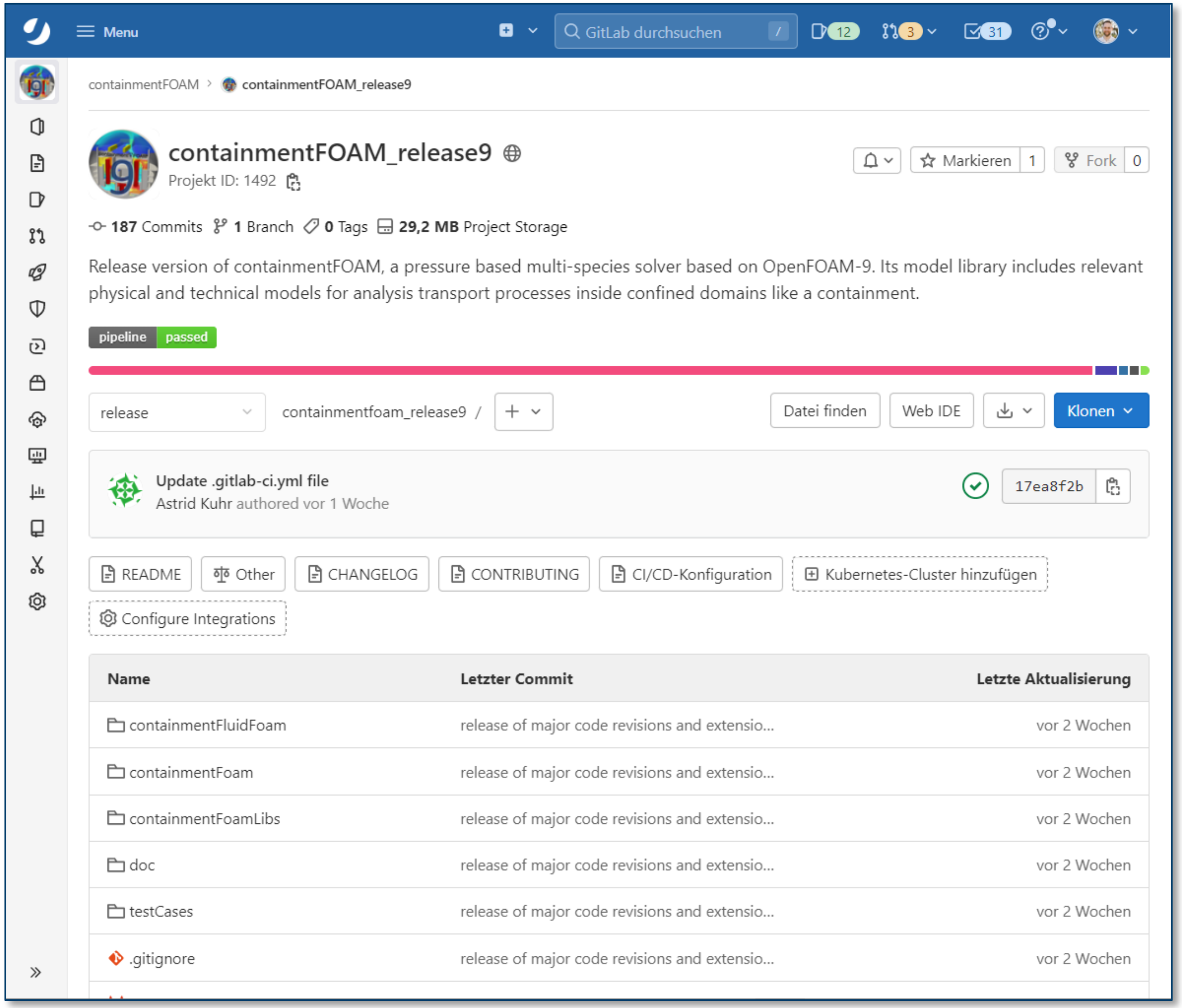
OUTLINE

- Severe Accidents and Containment Analysis
- Development of containment∇FOAM
- Theoretical Background
  - Buoyancy driven turbulent multi-species flows
  - Condensation processes
  - Thermal radiation
  - System models (PARs, code coupling, burst discs, porous models)
- containment∇FOAM framework
  - repository
  - cfGUI and cfSolutionMonitor
- Summary and Conclusions

CONTAINMENTFOAM REPOSITORY

Collaboration and Software Development Tools

- GitLab Platform at FZJ
  - Version management
  - CI/CD Environment
  - Ticket system
  - Wiki
  - flexible account management via ‚github accounts'



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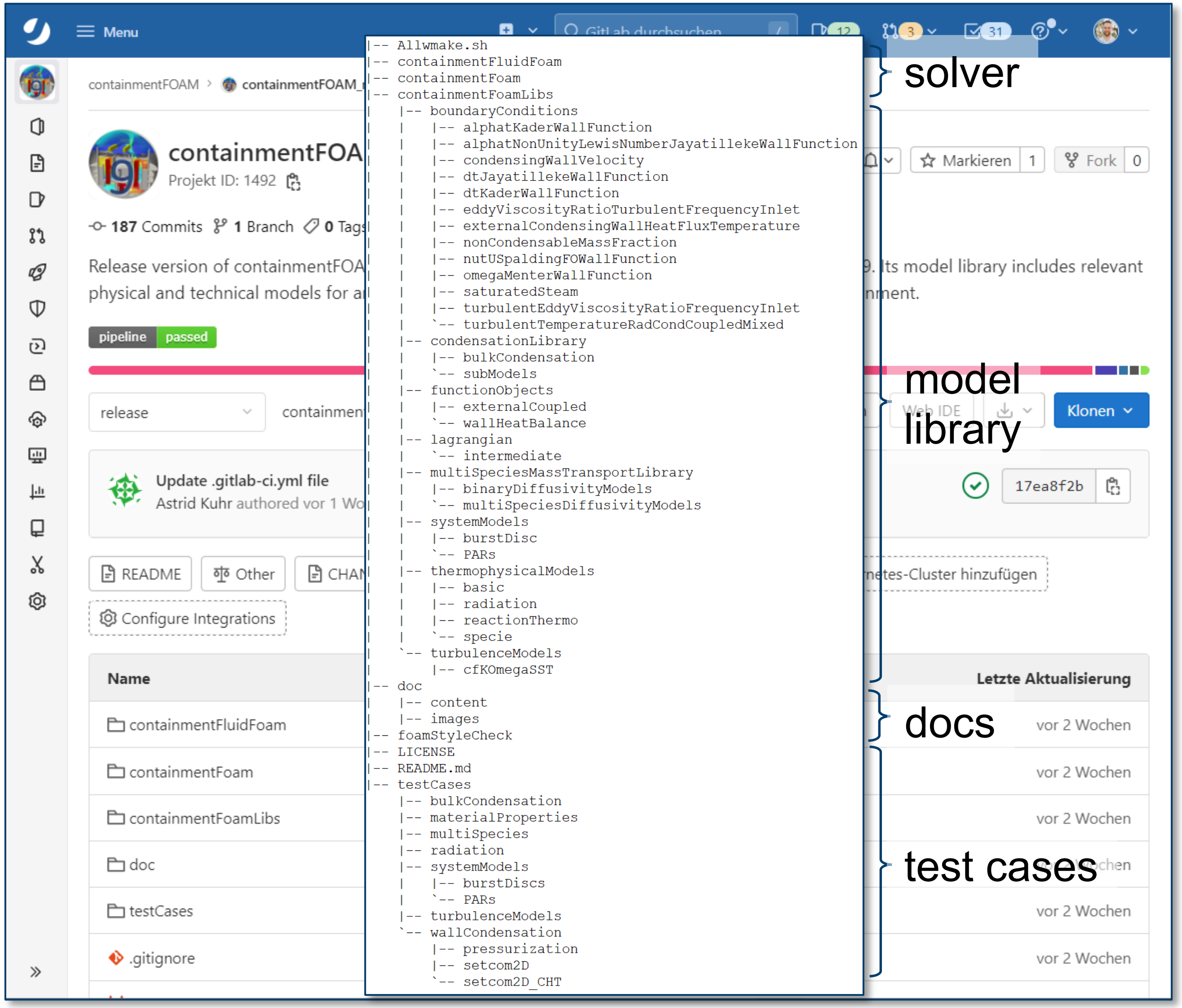

CONTAINMENTFOAM REPOSITORY

Documentation

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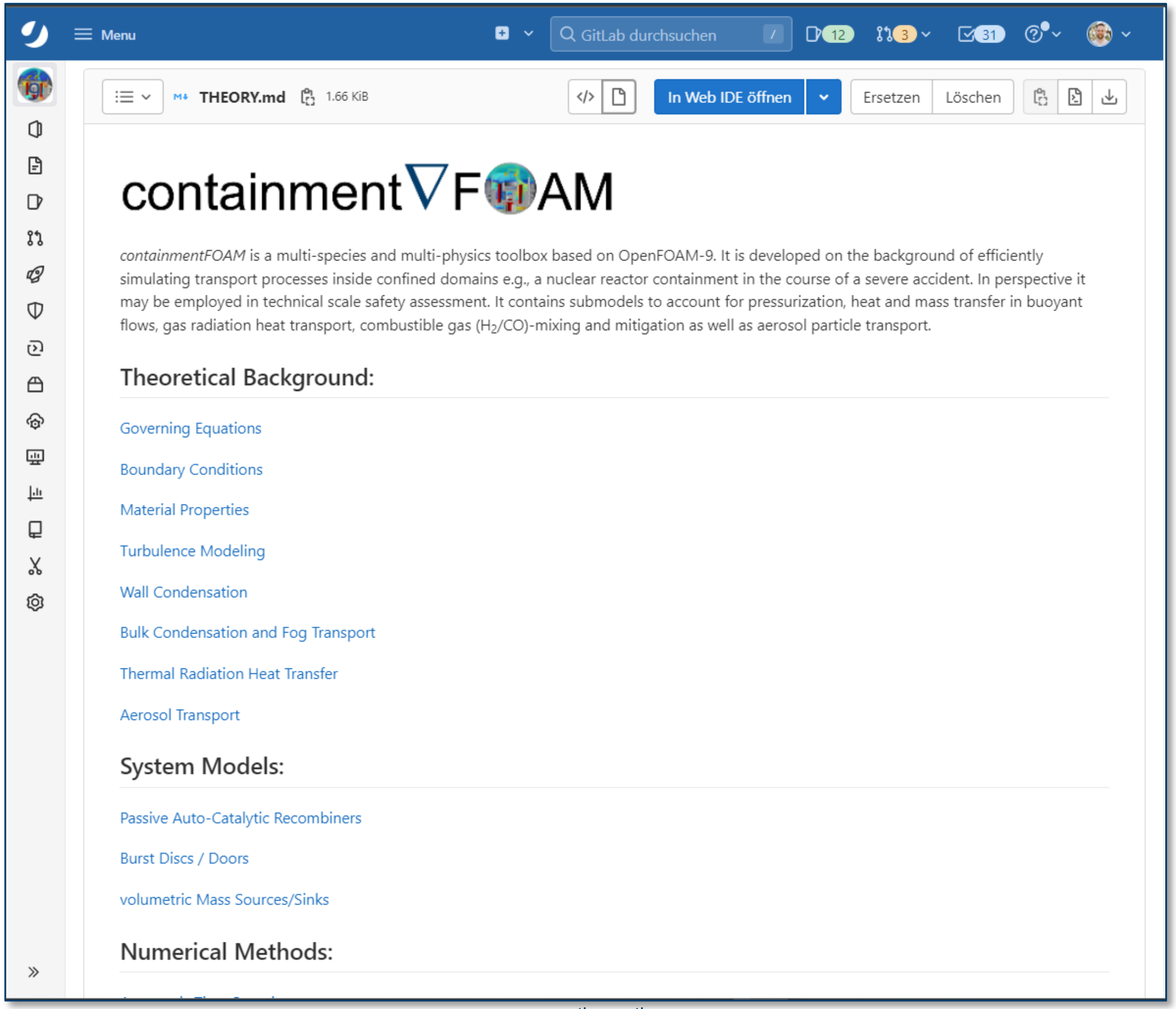

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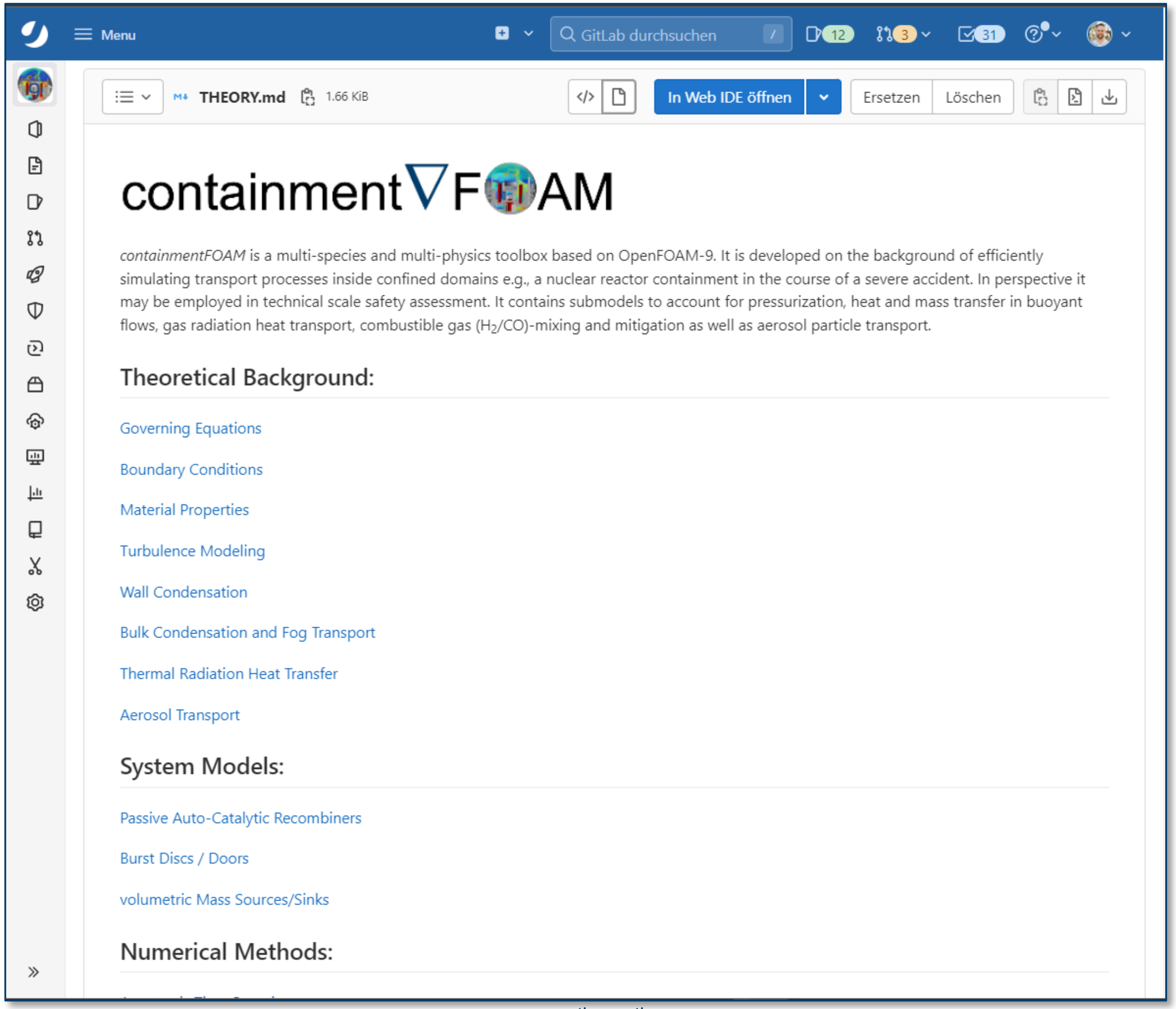

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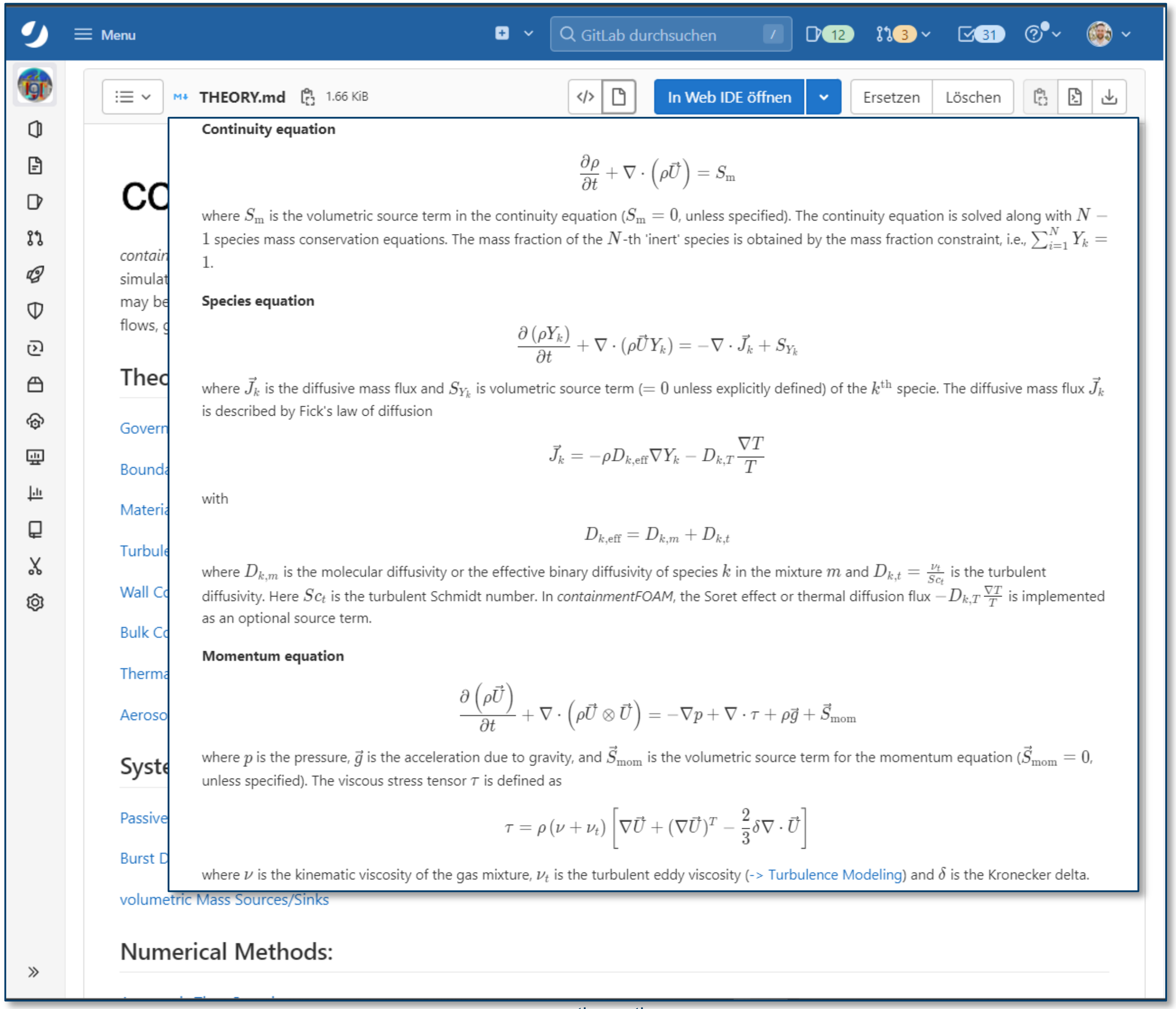
  - Solver description



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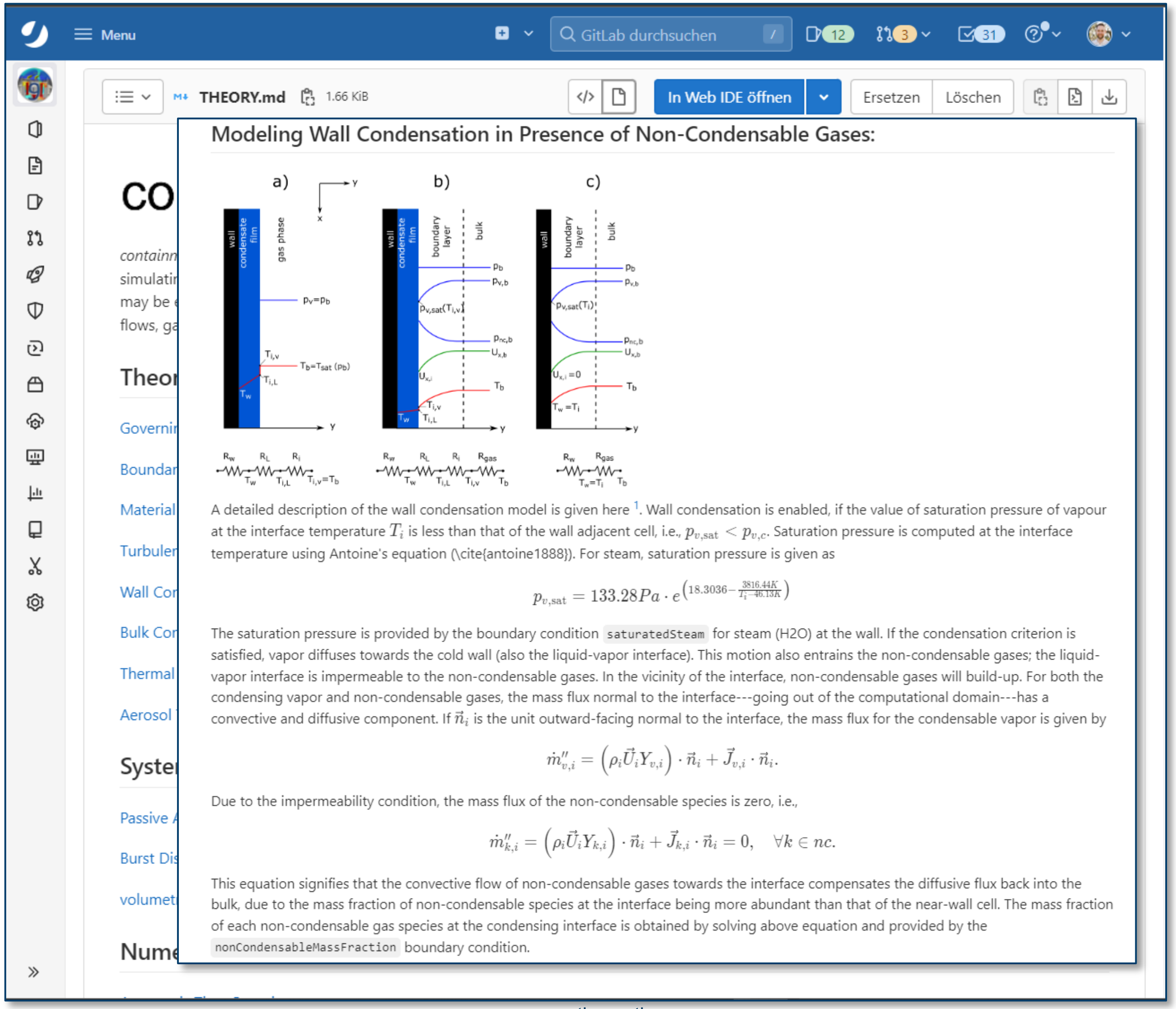

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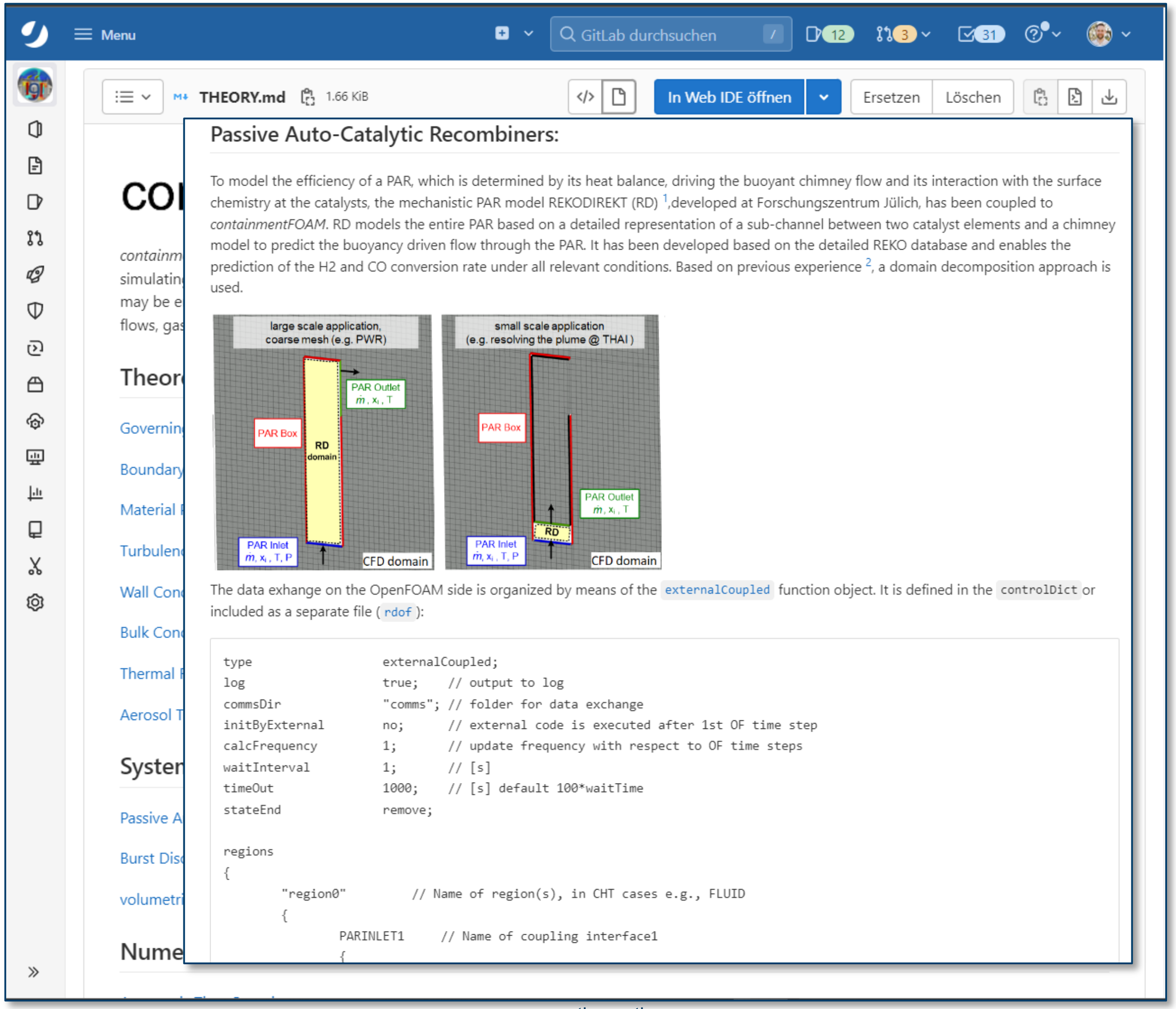

CONTAINMENTFOAM REPOSITORY

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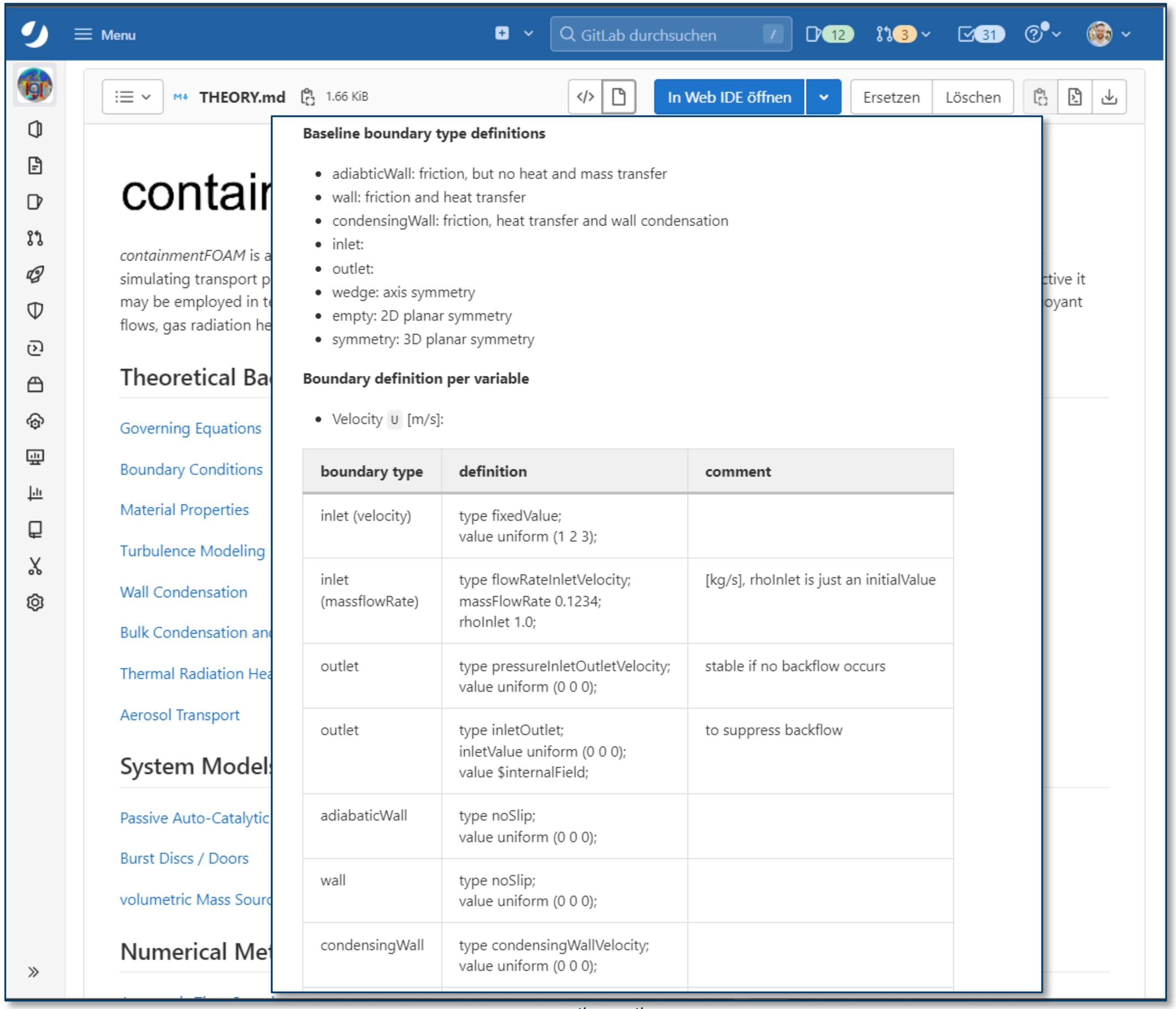
Documentation

- GitLab flavored Markdown files
  - Solver description
  - Modeling details
  - Standard boundary conditions



CONTAINMENTFOAM REPOSITORY

Documentation

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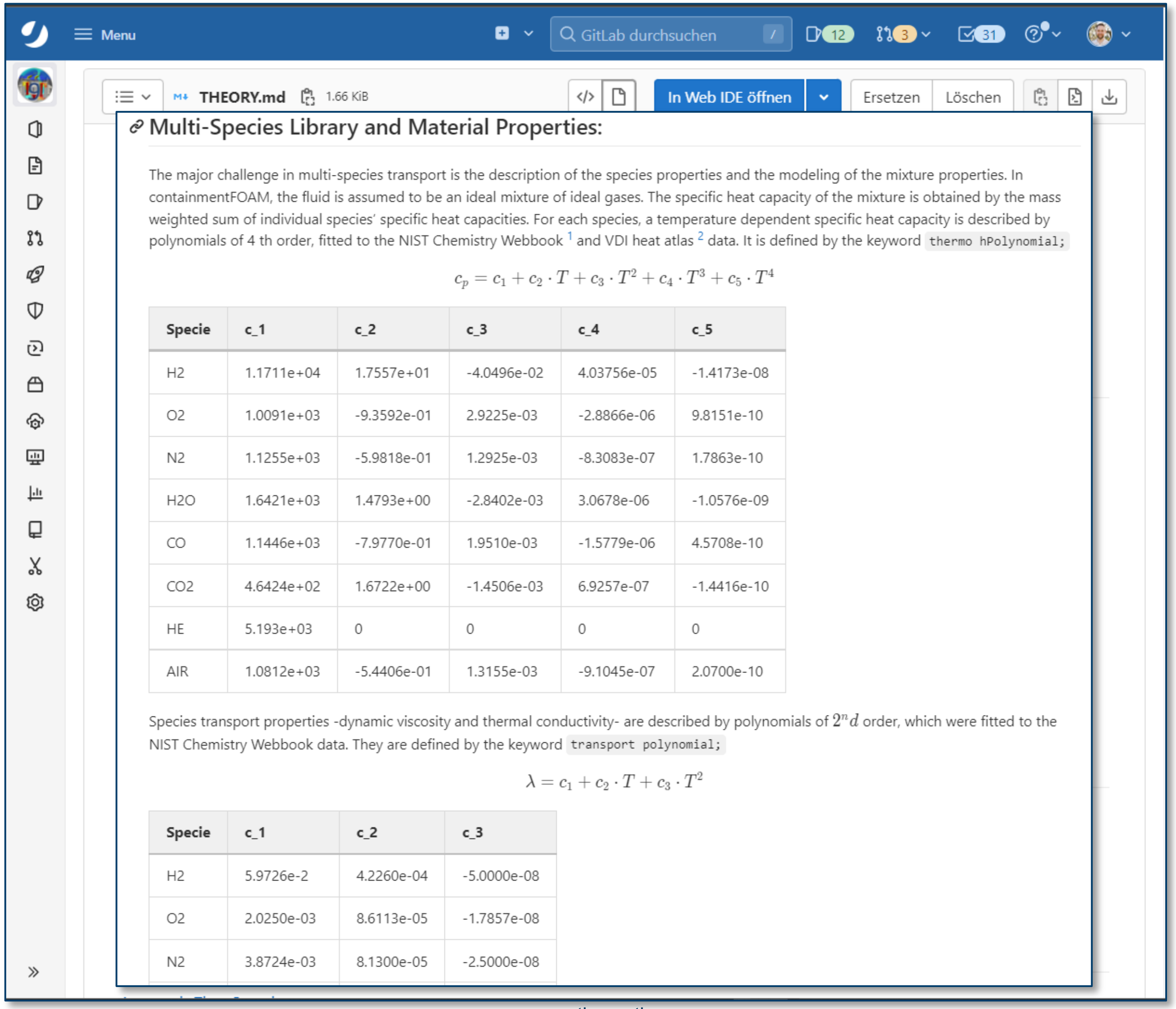
  - Modeling details
  - Standard boundary conditions
  - Material properties



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Multi-Species Library and Material Properties:

The major challenge in multi-species transport is the description of the species properties and the modeling of the mixture properties. In containmentFOAM, the fluid is assumed to be an ideal mixture of ideal gases. The specific heat capacity of the mixture is obtained by the mass weighted sum of individual species' specific heat capacities. For each species, a temperature dependent specific heat capacity is described by polynomials of 4 th order, fitted to the NIST Chemistry Webbook [1] and VDI heat atlas [2] data. It is defined by the keyword `thermo hPolynomial;`

$$c_p = c_1 + c_2 \cdot T + c_3 \cdot T^2 + c_4 \cdot T^3 + c_5 \cdot T^4$$

Specie	c_1	c_2	c_3	c_4	c_5
H2	1.1711e+04	1.7557e+01	-4.0496e-02	4.03756e-05	-1.4173e-08
O2	1.0091e+03	-9.3592e-01	2.9225e-03	-2.8866e-06	9.8151e-10
N2	1.1255e+03	-5.9818e-01	1.2925e-03	-8.3083e-07	1.7863e-10
H2O	1.6421e+03	1.4793e+00	-2.8402e-03	3.0678e-06	-1.0576e-09
CO	1.1446e+03	-7.9770e-01	1.9510e-03	-1.5779e-06	4.5708e-10
CO2	4.6424e+02	1.6722e+00	-1.4506e-03	6.9257e-07	-1.4416e-10
HE	5.193e+03	0	0	0	0
AIR	1.0812e+03	-5.4406e-01	1.3155e-03	-9.1045e-07	2.0700e-10

Species transport properties -dynamic viscosity and thermal conductivity- are described by polynomials of $2^n d$ order, which were fitted to the NIST Chemistry Webbook data. They are defined by the keyword `transport polynomial;`

$$\lambda = c_1 + c_2 \cdot T + c_3 \cdot T^2$$

Specie	c_1	c_2	c_3
H2	5.9726e-2	4.2260e-04	-5.0000e-08
O2	2.0250e-03	8.6113e-05	-1.7857e-08
N2	3.8724e-03	8.1300e-05	-2.5000e-08

CONTAINMENTFOAM REPOSITORY

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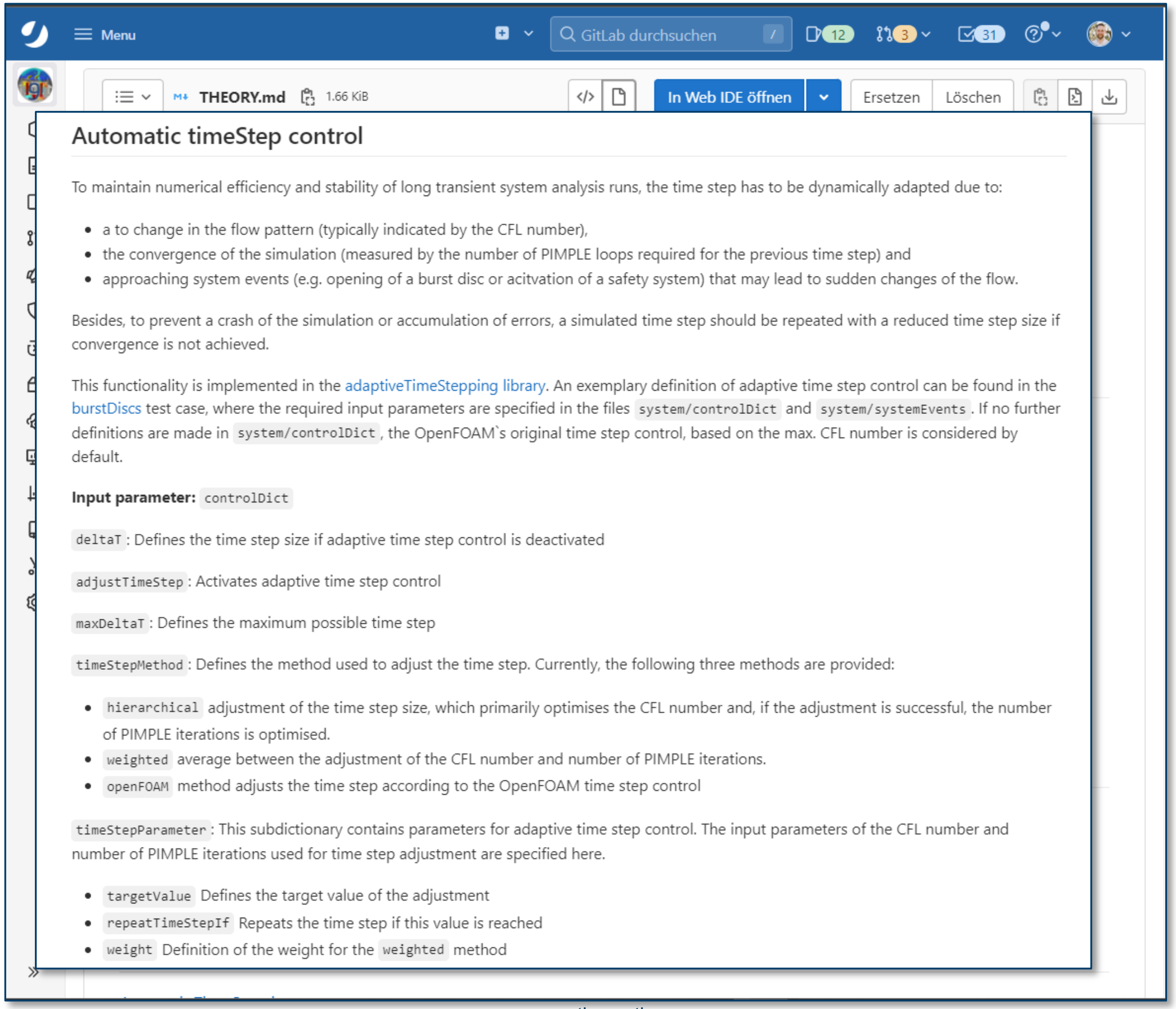
Documentation

- GitLab flavored Markdown files
  - Solver description
  - Modeling details
  - Standard boundary conditions
  - Material properties
  - Numerical methods



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Automatic timeStep control

To maintain numerical efficiency and stability of long transient system analysis runs, the time step has to be dynamically adapted due to:

- a to change in the flow pattern (typically indicated by the CFL number),
- the convergence of the simulation (measured by the number of PIMPLE loops required for the previous time step) and
- approaching system events (e.g. opening of a burst disc or acitvation of a safety system) that may lead to sudden changes of the flow.

Besides, to prevent a crash of the simulation or accumulation of errors, a simulated time step should be repeated with a reduced time step size if convergence is not achieved.

This functionality is implemented in the adaptiveTimeStepping library. An exemplary definition of adaptive time step control can be found in the burstDiscs test case, where the required input parameters are specified in the files `system/controlDict` and `system/systemEvents`. If no further definitions are made in `system/controlDict`, the OpenFOAM`s original time step control, based on the max. CFL number is considered by default.

Input parameter: `controlDict`

`deltaT`: Defines the time step size if adaptive time step control is deactivated

`adjustTimeStep`: Activates adaptive time step control

`maxDeltaT`: Defines the maximum possible time step

`timeStepMethod`: Defines the method used to adjust the time step. Currently, the following three methods are provided:

- `hierarchical` adjustment of the time step size, which primarily optimises the CFL number and, if the adjustment is successful, the number of PIMPLE iterations is optimised.
- `weighted` average between the adjustment of the CFL number and number of PIMPLE iterations.
- `openFOAM` method adjusts the time step according to the OpenFOAM time step control

`timeStepParameter`: This subdictionary contains parameters for adaptive time step control. The input parameters of the CFL number and number of PIMPLE iterations used for time step adjustment are specified here.

- `targetValue` Defines the target value of the adjustment
- `repeatTimeStepIf` Repeats the time step if this value is reached
- `weight` Definition of the weight for the `weighted` method

CONTAINMENTFOAM REPOSITORY

Documentation

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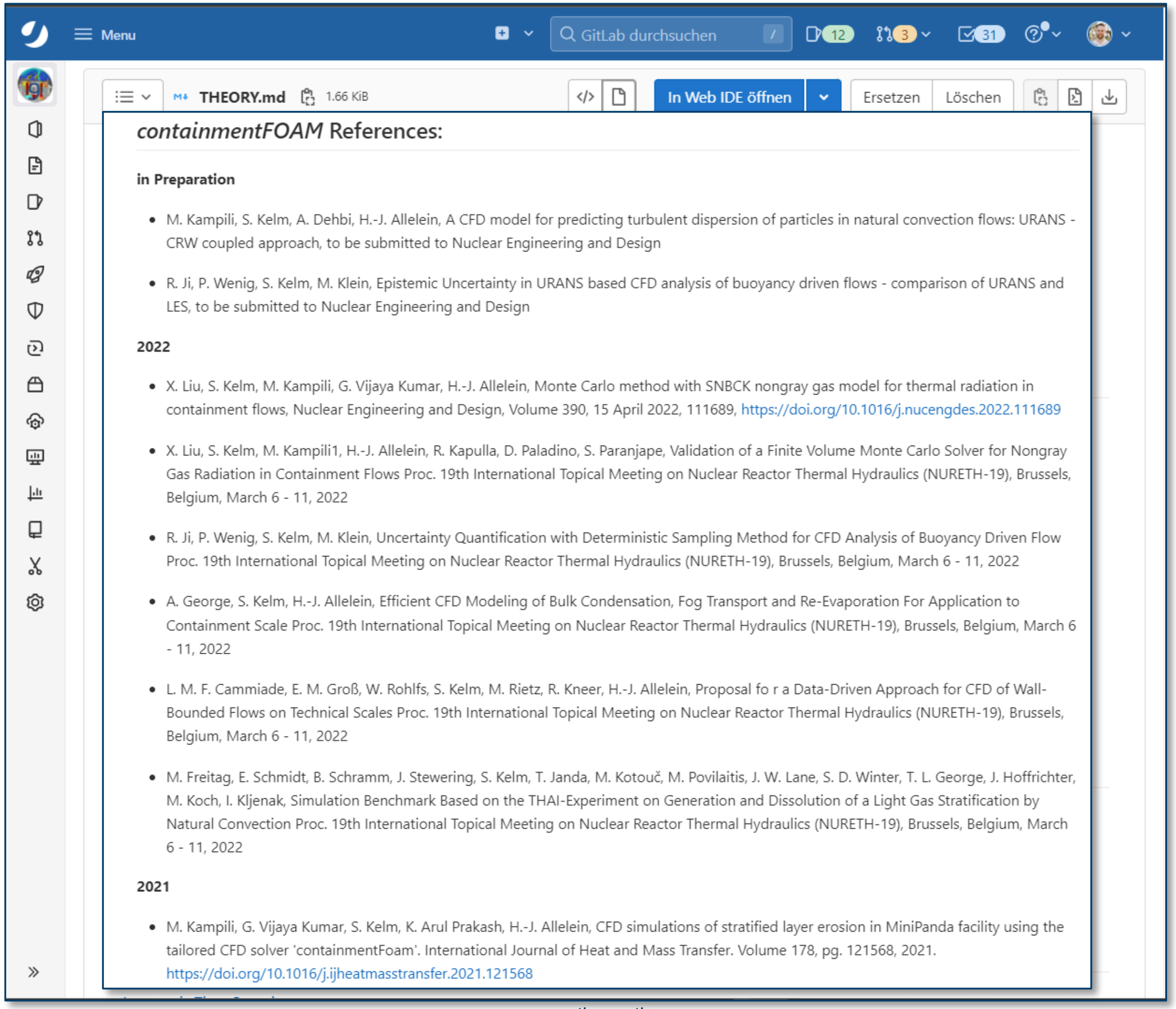
  - Standard boundary conditions
  - Material properties
  - Numerical methods
  - References



containmentFOAM References:

in Preparation

- M. Kampili, S. Kelm, A. Dehbi, H.-J. Allelein, A CFD model for predicting turbulent dispersion of particles in natural convection flows: URANS - CRW coupled approach, to be submitted to Nuclear Engineering and Design
- R. Ji, P. Wenig, S. Kelm, M. Klein, Epistemic Uncertainty in URANS based CFD analysis of buoyancy driven flows - comparison of URANS and LES, to be submitted to Nuclear Engineering and Design

2022

- X. Liu, S. Kelm, M. Kampili, G. Vijaya Kumar, H.-J. Allelein, Monte Carlo method with SNBCK nongray gas model for thermal radiation in containment flows, Nuclear Engineering and Design, Volume 390, 15 April 2022, 111689, https://doi.org/10.1016/j.nucengdes.2022.111689
- X. Liu, S. Kelm, M. Kampili1, H.-J. Allelein, R. Kapulla, D. Paladino, S. Paranjape, Validation of a Finite Volume Monte Carlo Solver for Nongray Gas Radiation in Containment Flows Proc. 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19), Brussels, Belgium, March 6 - 11, 2022
- R. Ji, P. Wenig, S. Kelm, M. Klein, Uncertainty Quantification with Deterministic Sampling Method for CFD Analysis of Buoyancy Driven Flow Proc. 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19), Brussels, Belgium, March 6 - 11, 2022
- A. George, S. Kelm, H.-J. Allelein, Efficient CFD Modeling of Bulk Condensation, Fog Transport and Re-Evaporation For Application to Containment Scale Proc. 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19), Brussels, Belgium, March 6 - 11, 2022
- L. M. F. Cammiade, E. M. Groß, W. Rohlfs, S. Kelm, M. Rietz, R. Kneer, H.-J. Allelein, Proposal fo r a Data-Driven Approach for CFD of Wall-Bounded Flows on Technical Scales Proc. 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19), Brussels, Belgium, March 6 - 11, 2022
- M. Freitag, E. Schmidt, B. Schramm, J. Stewering, S. Kelm, T. Janda, M. Kotouč, M. Povilaitis, J. W. Lane, S. D. Winter, T. L. George, J. Hoffrichter, M. Koch, I. Kljenak, Simulation Benchmark Based on the THAI-Experiment on Generation and Dissolution of a Light Gas Stratification by Natural Convection Proc. 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19), Brussels, Belgium, March 6 - 11, 2022

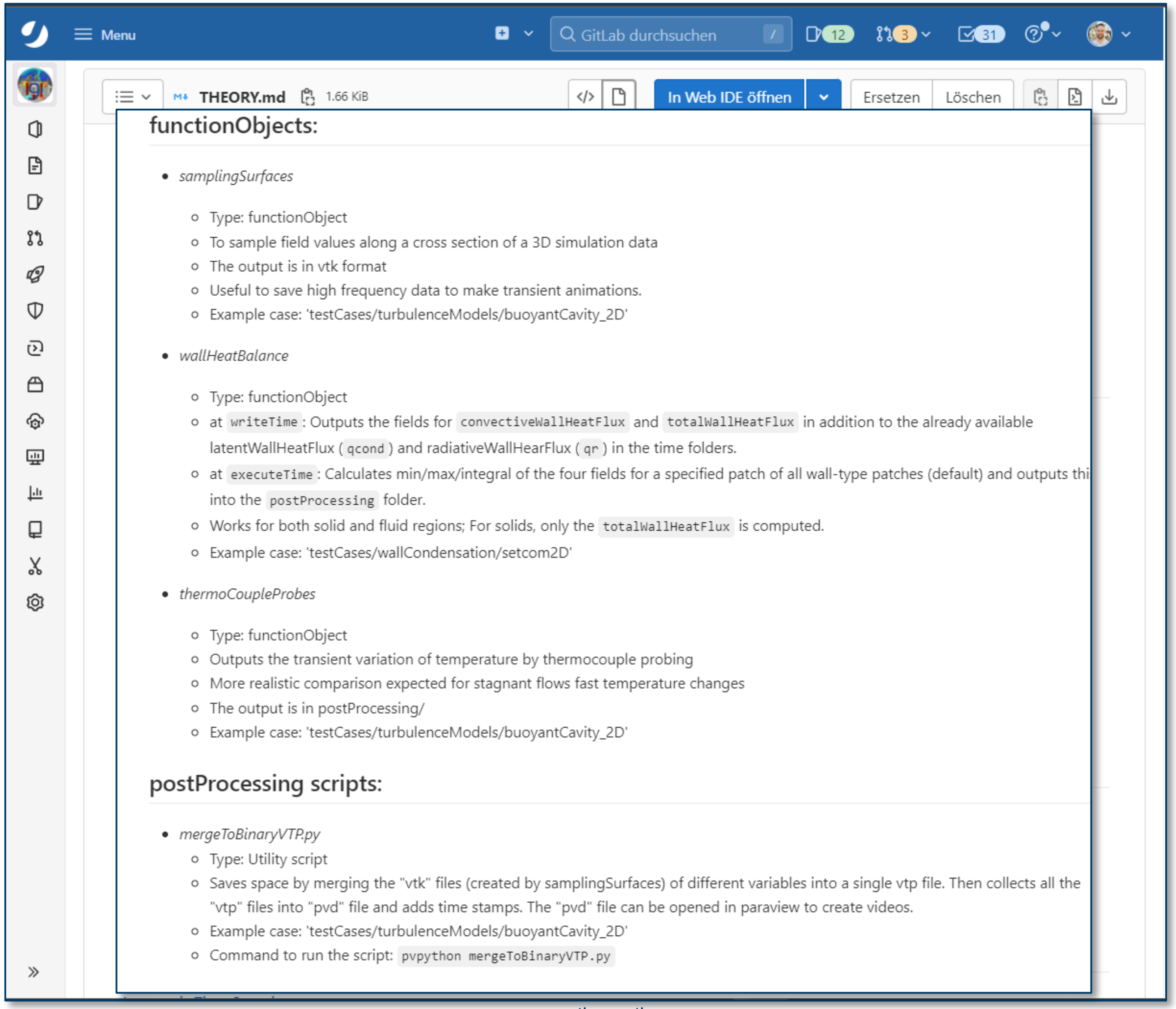
2021

- M. Kampili, G. Vijaya Kumar, S. Kelm, K. Arul Prakash, H.-J. Allelein, CFD simulations of stratified layer erosion in MiniPanda facility using the tailored CFD solver 'containmentFoam'. International Journal of Heat and Mass Transfer. Volume 178, pg. 121568, 2021. https://doi.org/10.1016/j.ijheatmasstransfer.2021.121568

CONTAINMENTFOAM REPOSITORY

Documentation

- GitLab flavored Markdown files
  - Solver description
  - Modeling details
  - Standard boundary conditions
  - Material properties
  - Numerical methods
  - References
  - Useful tools

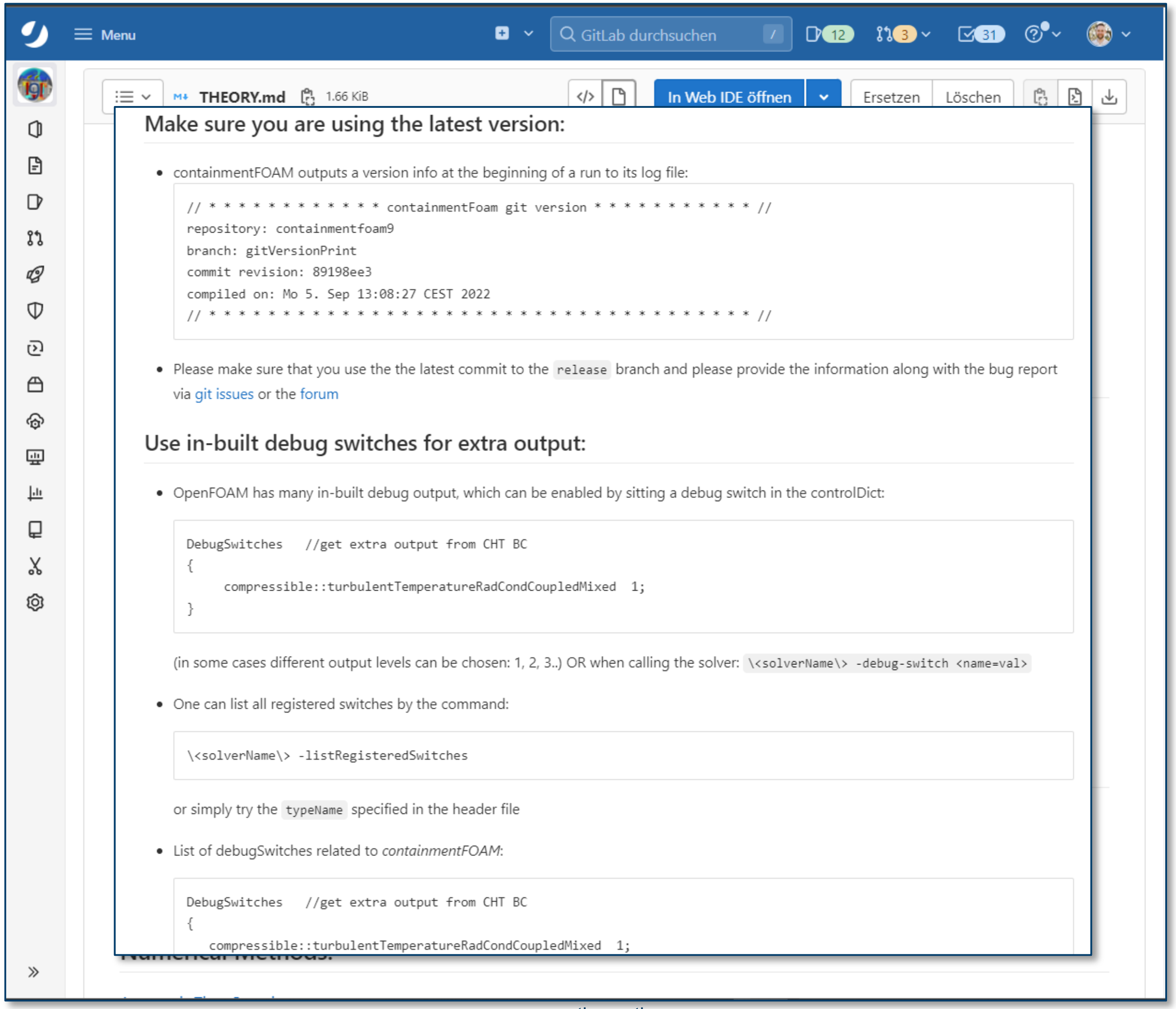


CONTAINMENTFOAM REPOSITORY

JÜLICH Forschungszentrum

Documentation

- GitLab flavored Markdown files
  - Solver description
  - Modeling details
  - Standard boundary conditions
  - Material properties
  - Numerical methods
  - References
  - Useful tools
  - Troubleshooting / Debugging



CONTAINMENTFOAM REPOSITORY

Documentation

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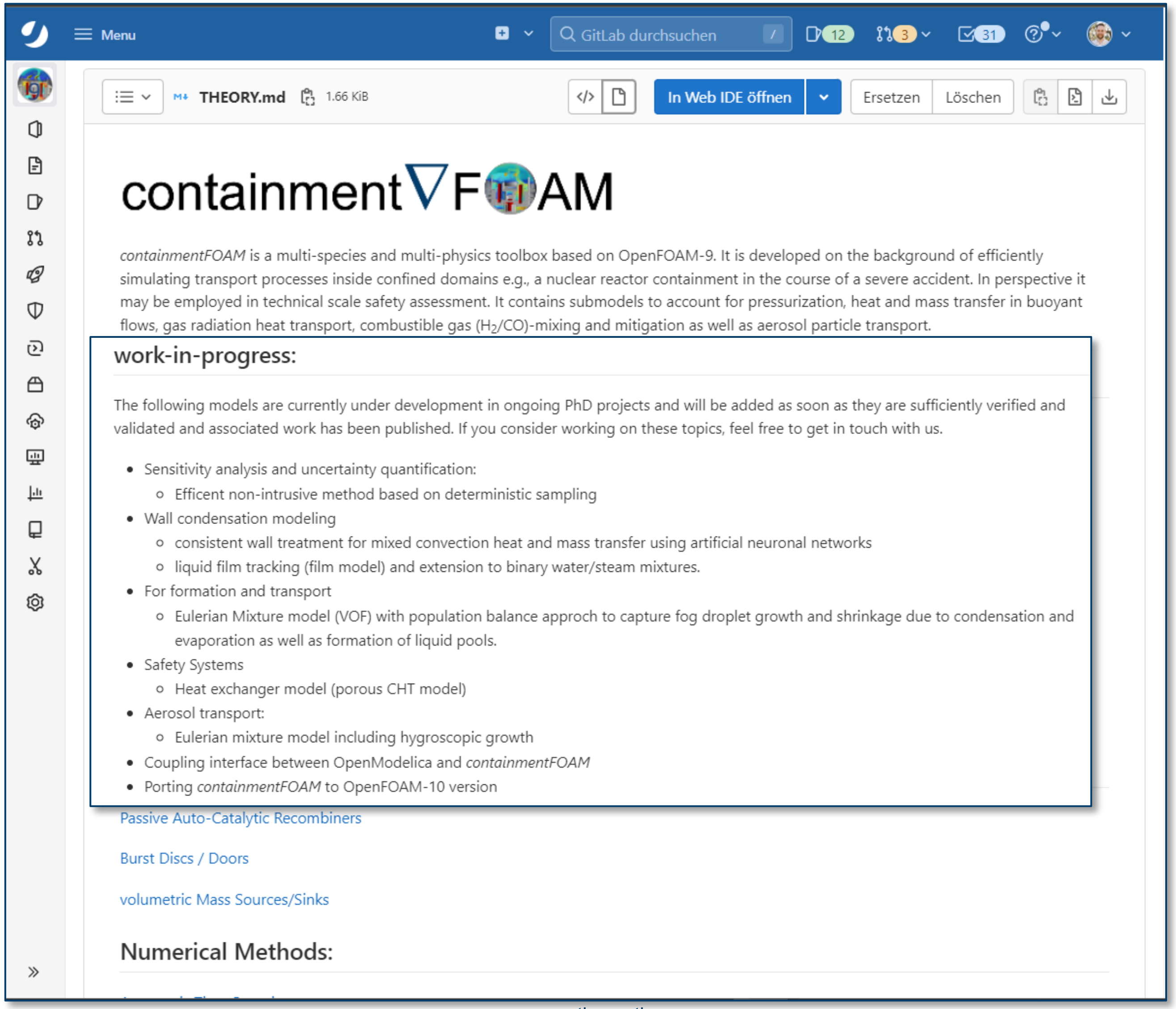
  - Numerical methods
  - References
  - Useful tools
  - Troubleshooting / Debugging
  - Work-in-Progress



CONTAINMENTFOAM REPOSITORY

Documentation

- GitLab flavored Markdown files
  - Solver description
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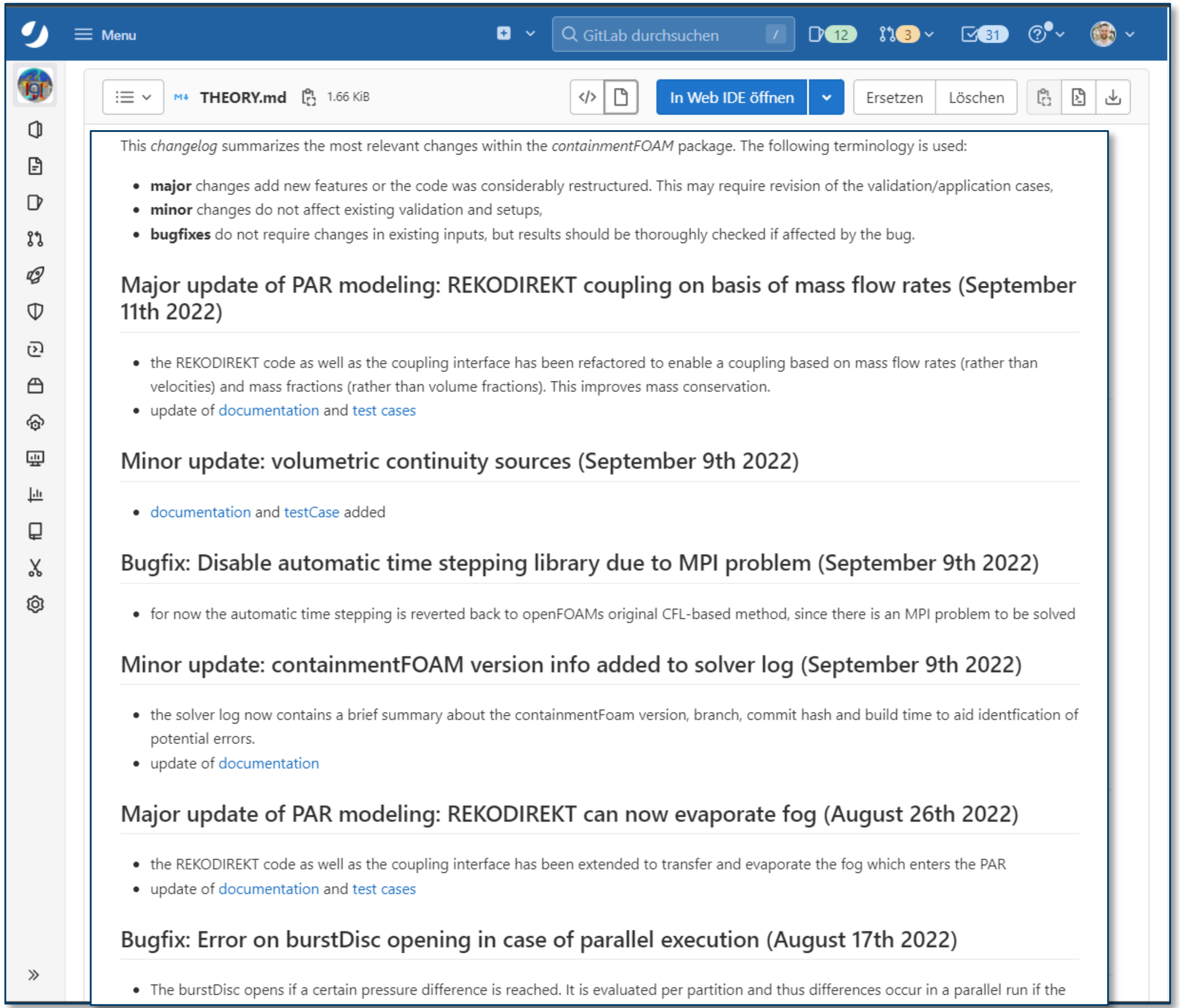
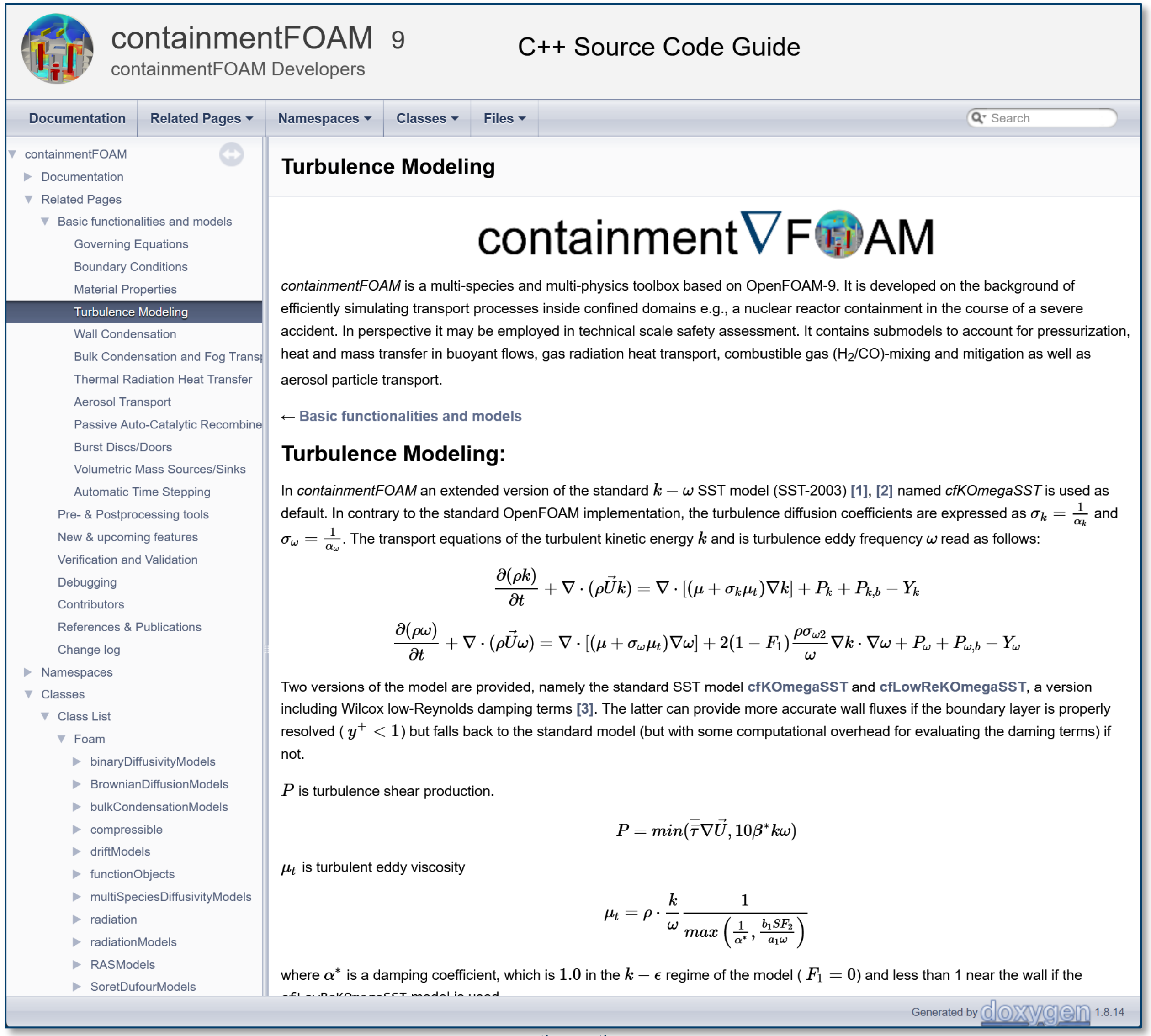
  - Numerical methods
  - References
  - Useful tools
  - Troubleshooting / Debugging
  - Work-in-Progress
  - Changelog



REPOSITORY

Collaboration and Software Development Tools

- GitLab Pages:
  - Automatic build of Doxygen documentation as web page hosted within the repository: https://containmentfoam_developers.iffgit.fz-juelich.de/containmentfoam_release9/index.html
  - Aims:
    - link markdown documentation and source


containmentFOAM 9
containmentFOAM Developers
C++ Source Code Guide

Documentation | Related Pages | Namespaces | Classes | Files | Search

- containmentFOAM
  - Documentation
  - Related Pages
    - Basic functionalities and models
      - Governing Equations
      - Boundary Conditions
      - Material Properties
      - Turbulence Modeling
      - Wall Condensation
      - Bulk Condensation and Fog Transp
      - Thermal Radiation Heat Transfer
      - Aerosol Transport
      - Passive Auto-Catalytic Recombine
      - Burst Discs/Doors
      - Volumetric Mass Sources/Sinks
      - Automatic Time Stepping
    - Pre- & Postprocessing tools
    - New & upcoming features
    - Verification and Validation
    - Debugging
    - Contributors
    - References & Publications
    - Change log
  - Namespaces
  - Classes
    - Class List
      - Foam
        - binaryDiffusivityModels
        - BrownianDiffusionModels
        - bulkCondensationModels
        - compressible
        - driftModels
        - functionObjects
        - multiSpeciesDiffusivityModels
        - radiation
        - radiationModels
        - RASModels
        - SoretDufourModels

Turbulence Modeling

containment∇FOAM

containmentFOAM is a multi-species and multi-physics toolbox based on OpenFOAM-9. It is developed on the background of efficiently simulating transport processes inside confined domains e.g., a nuclear reactor containment in the course of a severe accident. In perspective it may be employed in technical scale safety assessment. It contains submodels to account for pressurization, heat and mass transfer in buoyant flows, gas radiation heat transport, combustible gas (H_2/CO)-mixing and mitigation as well as aerosol particle transport.

← Basic functionalities and models

Turbulence Modeling:

In *containmentFOAM* an extended version of the standard $k-\omega$ SST model (SST-2003) [1], [2] named *cfKOmegaSST* is used as default. In contrary to the standard OpenFOAM implementation, the turbulence diffusion coefficients are expressed as $\sigma_k = \frac{1}{\alpha_k}$ and $\sigma_\omega = \frac{1}{\alpha_\omega}$. The transport equations of the turbulent kinetic energy k and is turbulence eddy frequency ω read as follows:

$$\frac{\partial(\rho k)}{\partial t} + \nabla\cdot(\rho\vec{U}k) = \nabla\cdot[(\mu+\sigma_k\mu_t)\nabla k] + P_k + P_{k,b} - Y_k$$

$$\frac{\partial(\rho\omega)}{\partial t} + \nabla\cdot(\rho\vec{U}\omega) = \nabla\cdot[(\mu+\sigma_\omega\mu_t)\nabla\omega] + 2(1-F_1)\frac{\rho\sigma_{\omega 2}}{\omega}\nabla k\cdot\nabla\omega + P_\omega + P_{\omega,b} - Y_\omega$$

Two versions of the model are provided, namely the standard SST model **cfKOmegaSST** and **cfLowReKOmegaSST**, a version including Wilcox low-Reynolds damping terms [3]. The latter can provide more accurate wall fluxes if the boundary layer is properly resolved ($y^+ < 1$) but falls back to the standard model (but with some computational overhead for evaluating the daming terms) if not.

P is turbulence shear production.

$$P = min(\bar{\tau}\nabla\vec{U}, 10\beta^* k\omega)$$

μ_t is turbulent eddy viscosity

$$\mu_t = \rho\cdot\frac{k}{\omega}\frac{1}{max\left(\frac{1}{\alpha^*}, \frac{b_1 SF_2}{a_1\omega}\right)}$$

where α^* is a damping coefficient, which is 1.0 in the $k-\epsilon$ regime of the model ($F_1 = 0$) and less than 1 near the wall if the

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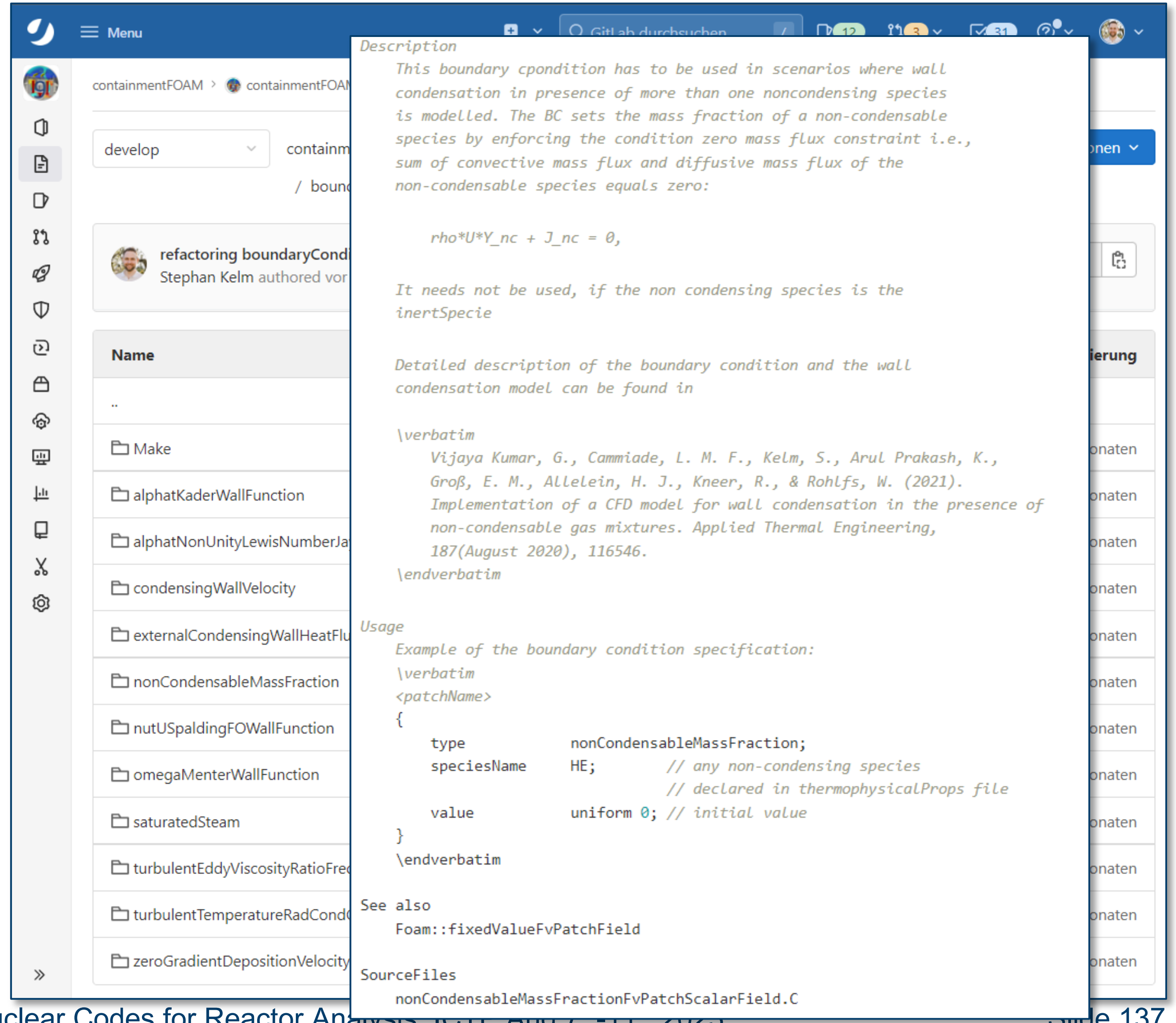
CONTAINMENTFOAM REPOSITORY

Documentation

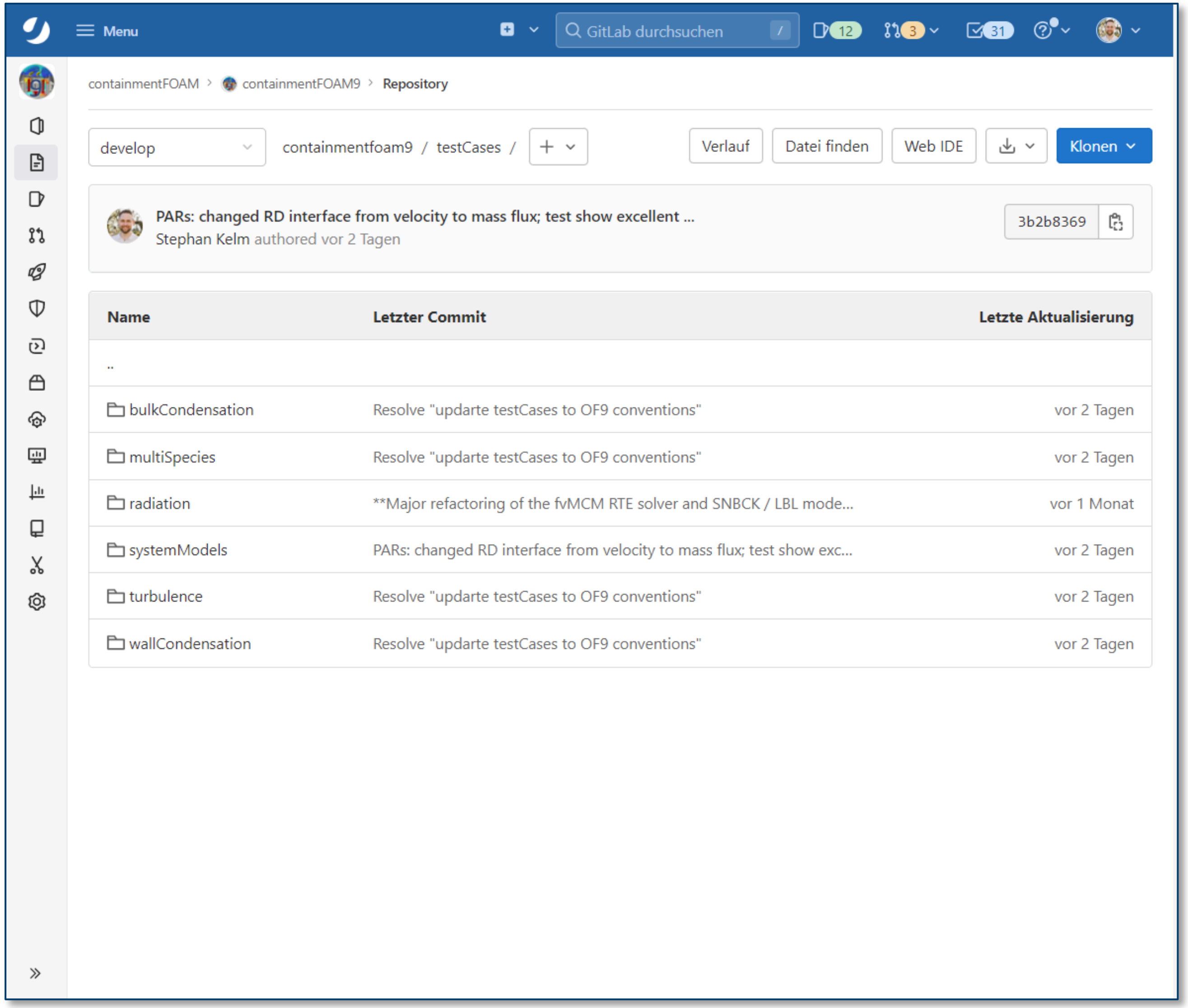
- Source code header files



CONTAINMENTFOAM REPOSITORY

TestCases

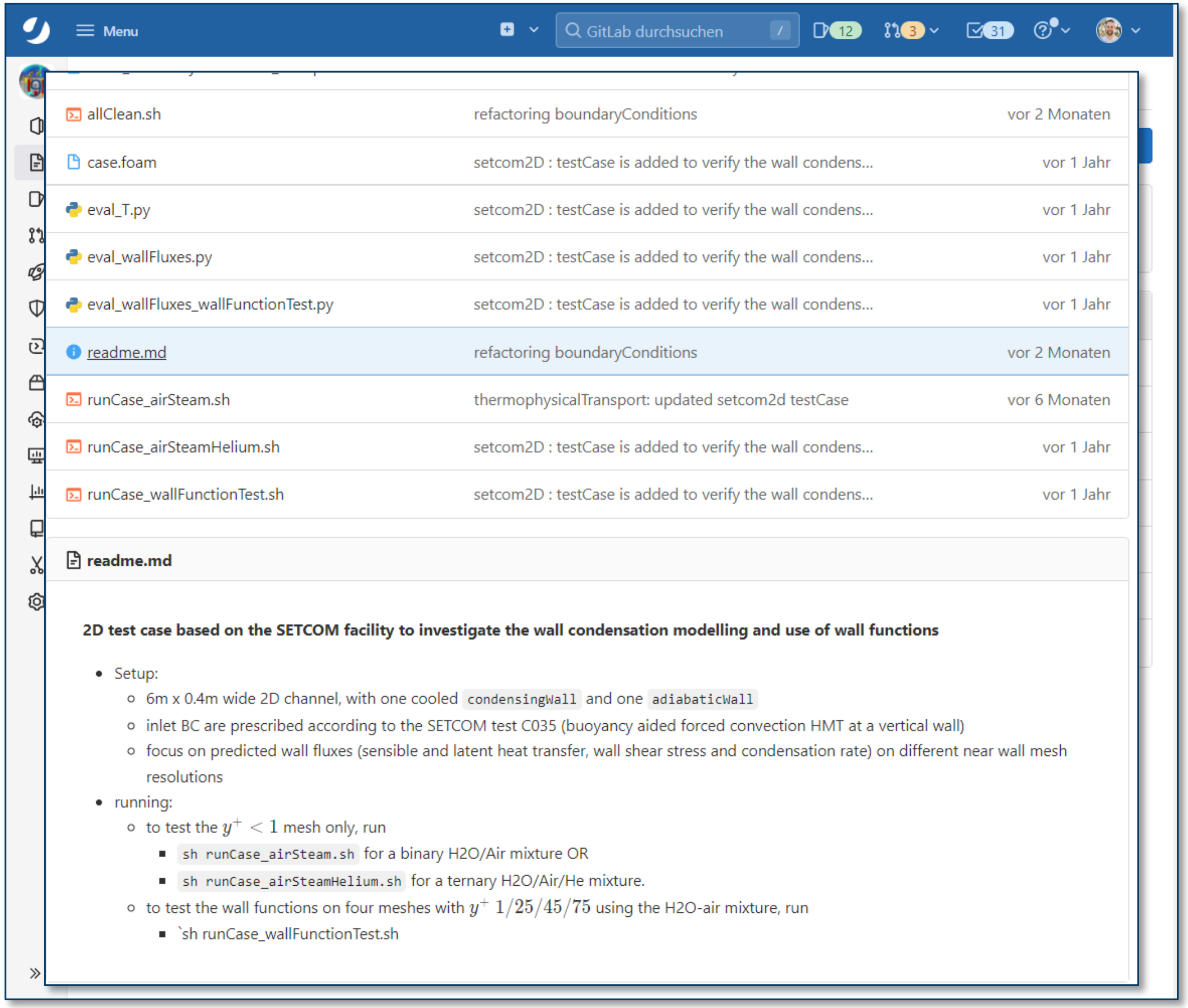
- Organized according to model library
- (Mostly) contain:
  - readme
  - run-script (several options possible)
  - reference data
  - postprocessing script



CONTAINMENTFOAM REPOSITORY

TestCases

- Organized according to model library
- (Mostly) contain:
  - readme
  - run-script (several options possible)
  - (link to) reference data
  - postprocessing script
- But in case of simple tests or demonstration no further information is provided.



CONTAINMENTFOAM REPOSITORY

Contributions

- Please help us maintaining containment∇FOAM rather than fork!
- Become a project member (issue tracker, notifications..)
- You developed a feature that could complement containment∇FOAM?

  (1) Check contribution guidelines

  (2) Get in touch with us (forum, email)

  (3) Two options:

    - Share code via a separate repository, which is linked
    - Merge code into containment∇FOAM repository
- You identified a potential bug
  - Raise an issue and provide a description and testCase
- Propose extensions, test cases, review

containmentFOAM Contribution guidelines:

- If you wish to develop/have a new feature, please get in touch with us via email to discuss its integration.
- Create an issue with a consolidated title and sufficient description. Assign the person resposible (if known), while creating the issue itself.
- To address the issue rised in code development, the assigned person should create a branch and merge request using the option from issue itself. Care should be taken that the *parent branch is develop* (not master), as most recent developments are merged with it. By default, this creates a branch name starting with "issue-number" and merge request with "Draft:" in front.
- Do not push images (plots) into the git. The verification plots, to prove the developed code in the branch works as intended, should be discussed in the comments section of the relevant merge-request.
- If there is a long standing bug in a specific part of the code, you may start a thread instead of comment in the associated merge-request, which allows a separate discussion.
- When the code is verified and ready to be merged with develop branch, remove the "Draft:" from merge-request and add the assignee reviewer. The reviewer can provide his approval for merging, and it is optional. The assignee should verify compilation, verification discussion in the comments section, and resolve the merge-conflicts,and finally merge with *develop* branch.
- Pushing commits into *develop* and *master* branches is strictly forbidden.
- *containmentFOAM* is developed under the GNU General Public Licence v3. The act of pushing code to the repository will be understood as an explicit affirmation of the following:
  - The contribution was created in whole or in part by me and I have the right to submit it under the GPL v3 (or the indicated compatible license)
  - My contribution is based upon previous work that, to the best of my knowledge, is covered under the GPL v3 (or the indicated compatible license) and I have the right to submit that work with modifications, under the same open source license, as indicated in the file; Or the contribution was provided directly to me by another person who certified the points above and I have not modified it.
  - My individual contribution is visible in the commit history and globally mentioned in above contributors list. Individual copyright statements should not be added to the source code

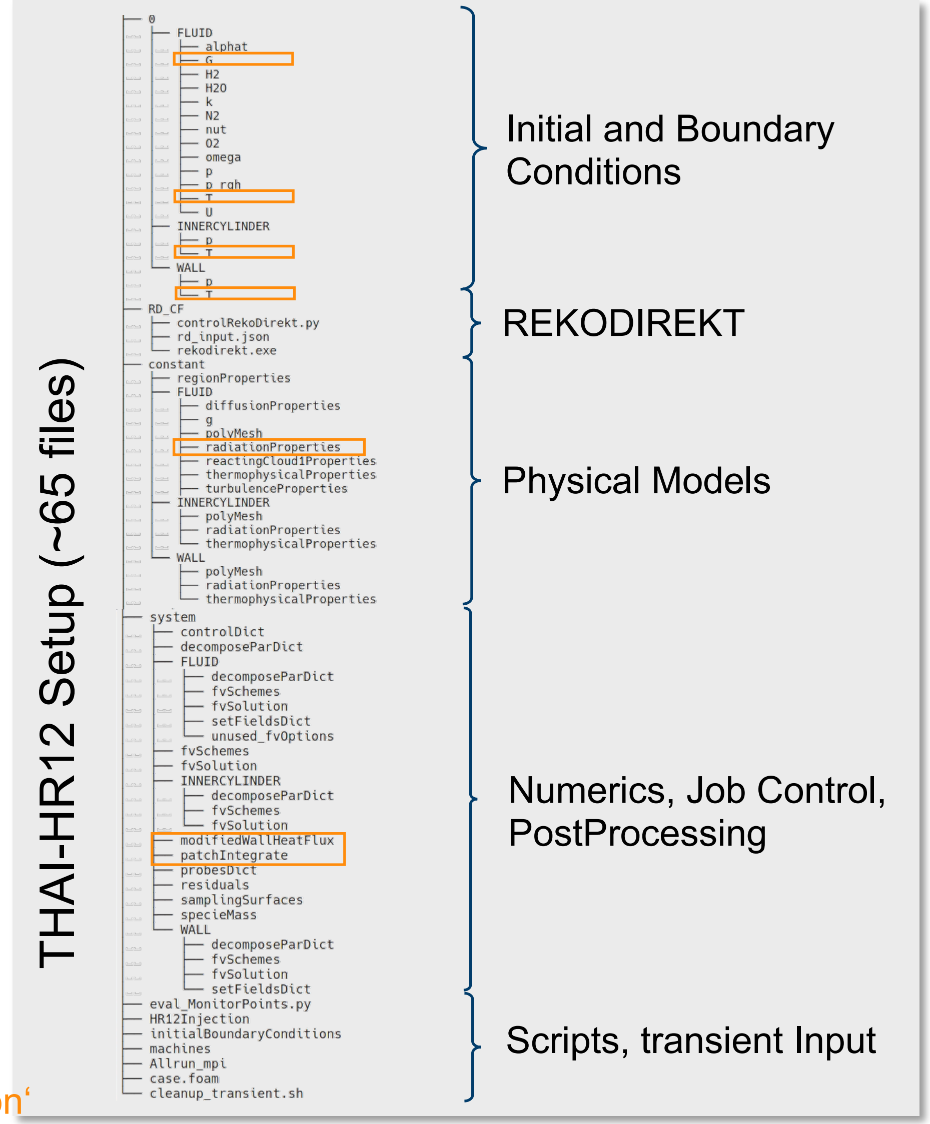
CONTAINMENTFOAM FRAMEWORK

Crosscutting issues – Case creation

- Containment analysis comprises interaction of multiple physical phenomena and safety systems:
  - Multiple specialized model options and defaults (developers experience)
  - Dependencies among dictionaries (and models)
- Different users, different approaches:
  - Broad variety of numerical methods and schemes
  - Different usage of OF-functionality

➢ Limited repeatability

➢ Inconsistent definitions possible, which may not cause a crash



Definition ‚gas radiation‘

CONTAINMENTFOAM FRAMEWORK

Crosscutting issues – Case creation

- E.g. inconsistent definitions possible, which may not cause a crash:
  - CHT boundary condition:

0/FLUID/T

```
INNERWALL {
   type     compressible::turbulentTemperatureRadCoupledMixed;
   Tnbr              T;
   kappaMethod       fluidThermo;
   kappa             kappa;
   qrNbr             none;
   qr                qr;
   qcondNbr          none;
   qcond             qcond; }
```

0/WALL/T

```
INNERWALL {
   type     compressible::turbulentTemperatureRadCoupledMixed;
   Tnbr              T;
   kappaMethod       fluidThermo;
   kappa             kappa;
   qrNbr             qr;
   qr                none;
   qcondNbr          qcond;
   qcond             none; }
```

Definition ‚region interface'

THAI-HR12 Setup (~65 files)

```
├── 0
│   ├── FLUID
│   │   ├── alphat
│   │   ├── G
│   │   ├── H2
│   │   ├── H2O
│   │   ├── k
│   │   ├── N2
│   │   ├── nut
│   │   ├── O2
│   │   ├── omega
│   │   ├── p
│   │   ├── p_rgh
│   │   ├── T
│   │   └── U
│   ├── INNERCYLINDER
│   │   ├── p
│   │   └── T
│   └── WALL
│       ├── p
│       └── T
├── RD_CF
│   ├── controlRekoDirekt.py
│   ├── rd_input.json
│   └── rekodirekt.exe
├── constant
│   ├── regionProperties
│   ├── FLUID
│   │   ├── diffusionProperties
│   │   ├── g
│   │   ├── polyMesh
│   │   ├── radiationProperties
│   │   ├── reactingCloud1Properties
│   │   ├── thermophysicalProperties
│   │   └── turbulenceProperties
│   ├── INNERCYLINDER
│   │   ├── polyMesh
│   │   ├── radiationProperties
│   │   └── thermophysicalProperties
│   └── WALL
│       ├── polyMesh
│       ├── radiationProperties
│       └── thermophysicalProperties
├── system
│   ├── controlDict
│   ├── decomposeParDict
│   ├── FLUID
│   │   ├── decomposeParDict
│   │   ├── fvSchemes
│   │   ├── fvSolution
│   │   ├── setFieldsDict
│   │   └── unused_fvOptions
│   ├── fvSchemes
│   ├── fvSolution
│   ├── INNERCYLINDER
│   │   ├── decomposeParDict
│   │   ├── fvSchemes
│   │   └── fvSolution
│   ├── modifiedWallHeatFlux
│   ├── patchIntegrate
│   ├── probesDict
│   ├── residuals
│   ├── samplingSurfaces
│   ├── specieMass
│   └── WALL
│       ├── decomposeParDict
│       ├── fvSchemes
│       ├── fvSolution
│       └── setFieldsDict
├── eval_MonitorPoints.py
├── HR12Injection
├── initialBoundaryConditions
├── machines
├── Allrun_mpi
├── case.foam
└── cleanup_transient.sh
```

- 0: Initial and Boundary Conditions
- RD_CF: REKODIREKT
- constant: Physical Models
- system: Numerics, Job Control, PostProcessing
- remaining files: Scripts, transient Input

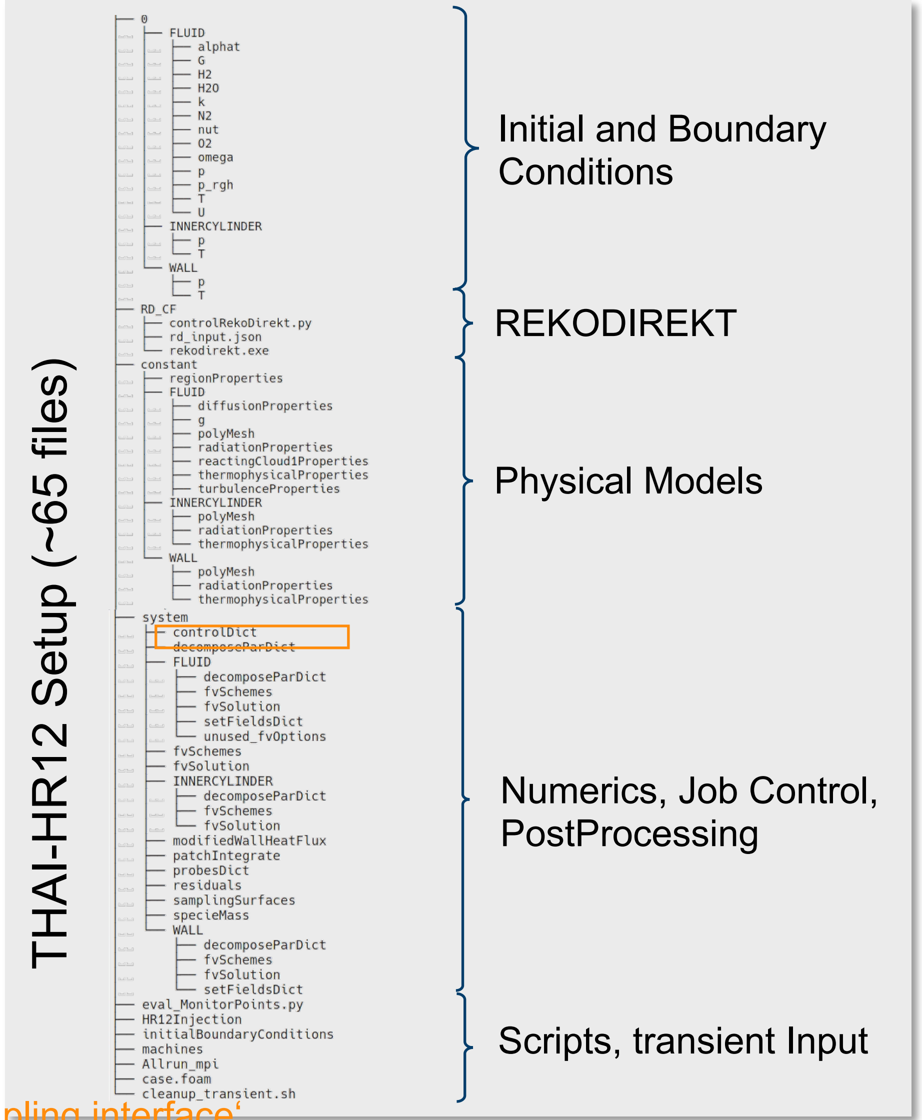
CONTAINMENTFOAM FRAMEWORK

Crosscutting issues – Case creation

- E.g. inconsistent definitions possible, which may not cause a crash:
  - Code coupling interface:

system/controlDict

```
type                    externalCoupled;
log                     false;
commsDir                "comms";
initByExternal          no;
calcFrequency           1;
stateEnd                remove;
regions {
    "region0" {
            PARINLET1 {
               readFields       (U);
               writeFields      (T O2 N2 H2O CO2 H2 CO p fog);
                           }
            PAROUTLET1 {
               readFields       (T U O2 N2 H2O CO2 H2 CO);
               writeFields      ();
}}}
```



Definition ‚coupling interface'

CONTAINMENTFOAM FRAMEWORK

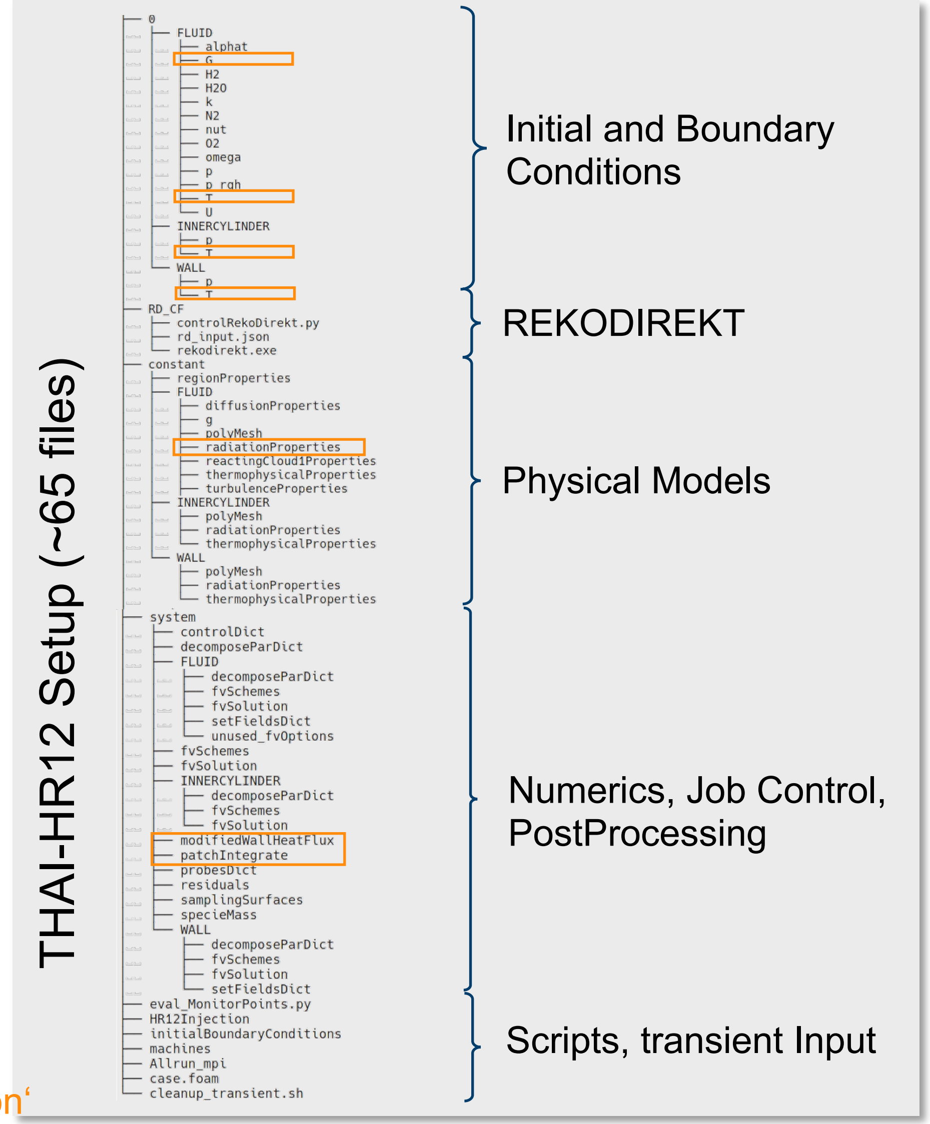
Crosscutting issues – Case creation

- Containment analysis comprises interaction of multiple physical phenomena and safety systems:
- Different users, different approaches
- Considerable syntax changes in OF base versions
- Reproduce preprocessing workflows

➢ ‚templated standard‘ & Best Practice required:

- Prevent input errors
- Ensure consistent model application
- Enable comparable and reproducible analysis
- Support / bug identification and fixing.

➢ Development of ‘cfGUI’



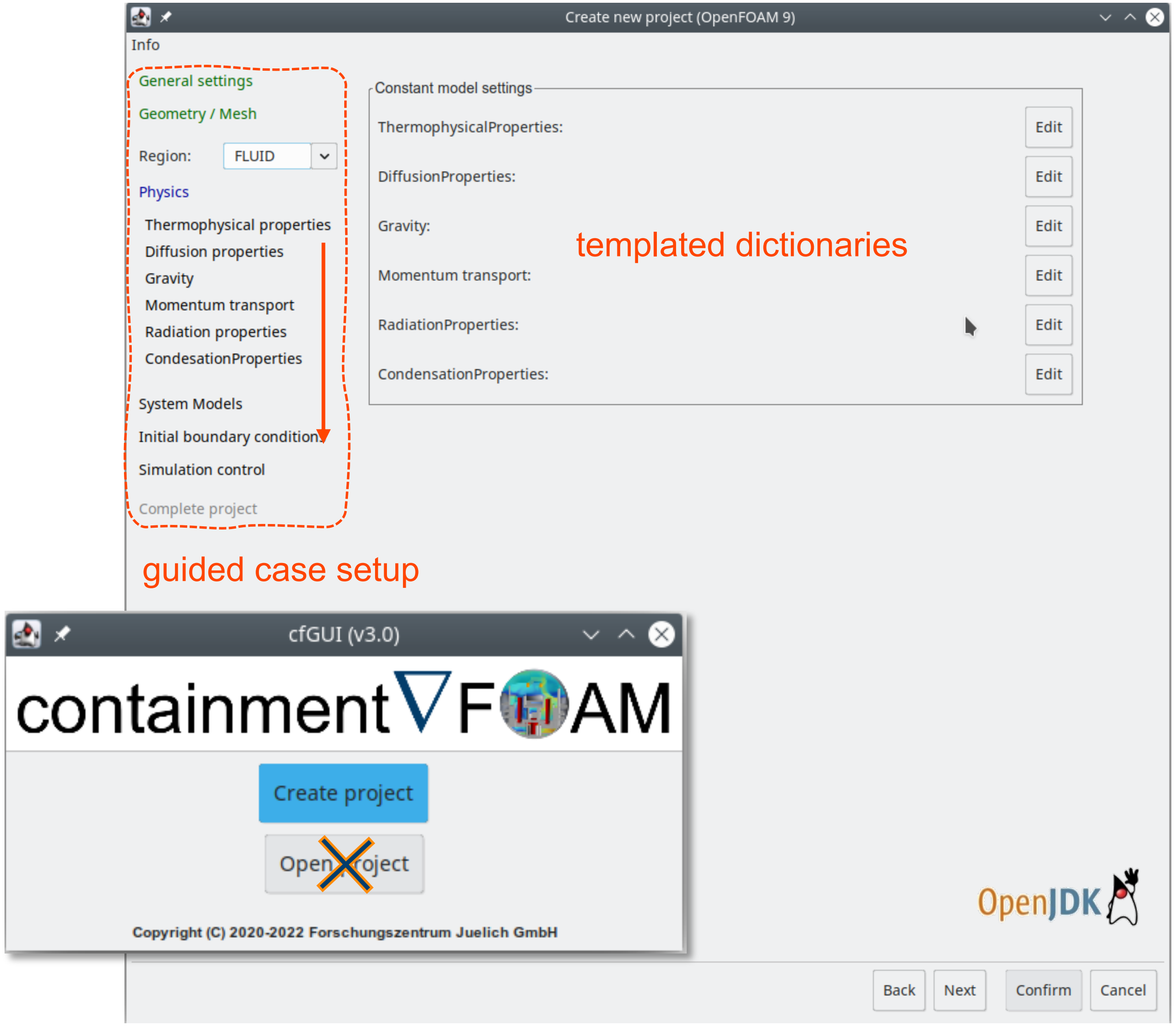
Definition ‚gas radiation‘

CONTAINMENTFOAM FRAMEWORK

Guided Case Setup

- Developed by two trainees during their Dual Curriculum MATSE + Applied Mathematics and Computer Science B.Sc.
  - ➢ Work in progress !!

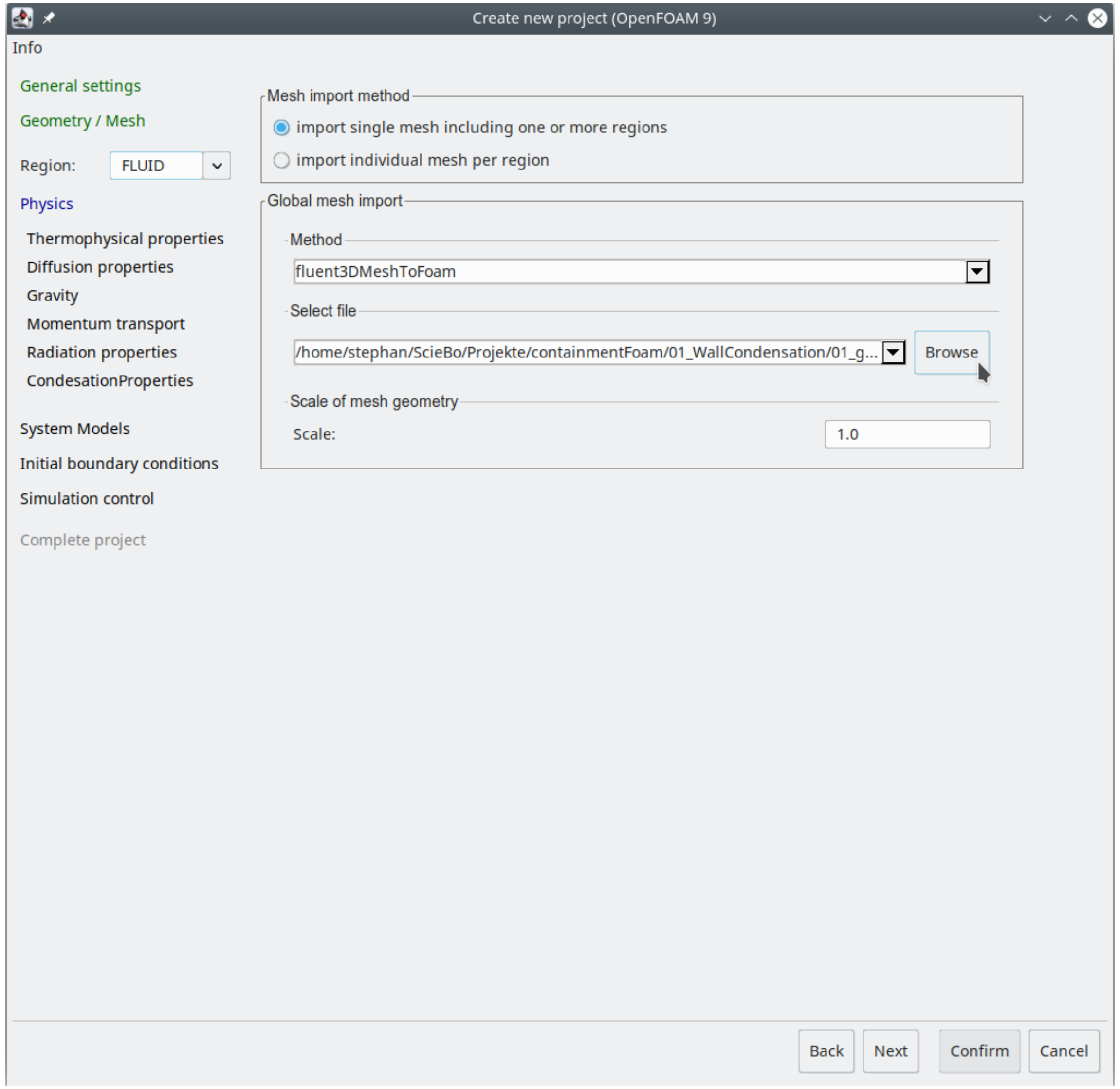
- General idea:
  - Workflow, structure and syntax close to OpenFOAM
  - limit functionality to baseline model and fundamental functionality



CONTAINMENTFOAM FRAMEWORK

Guided Case Setup

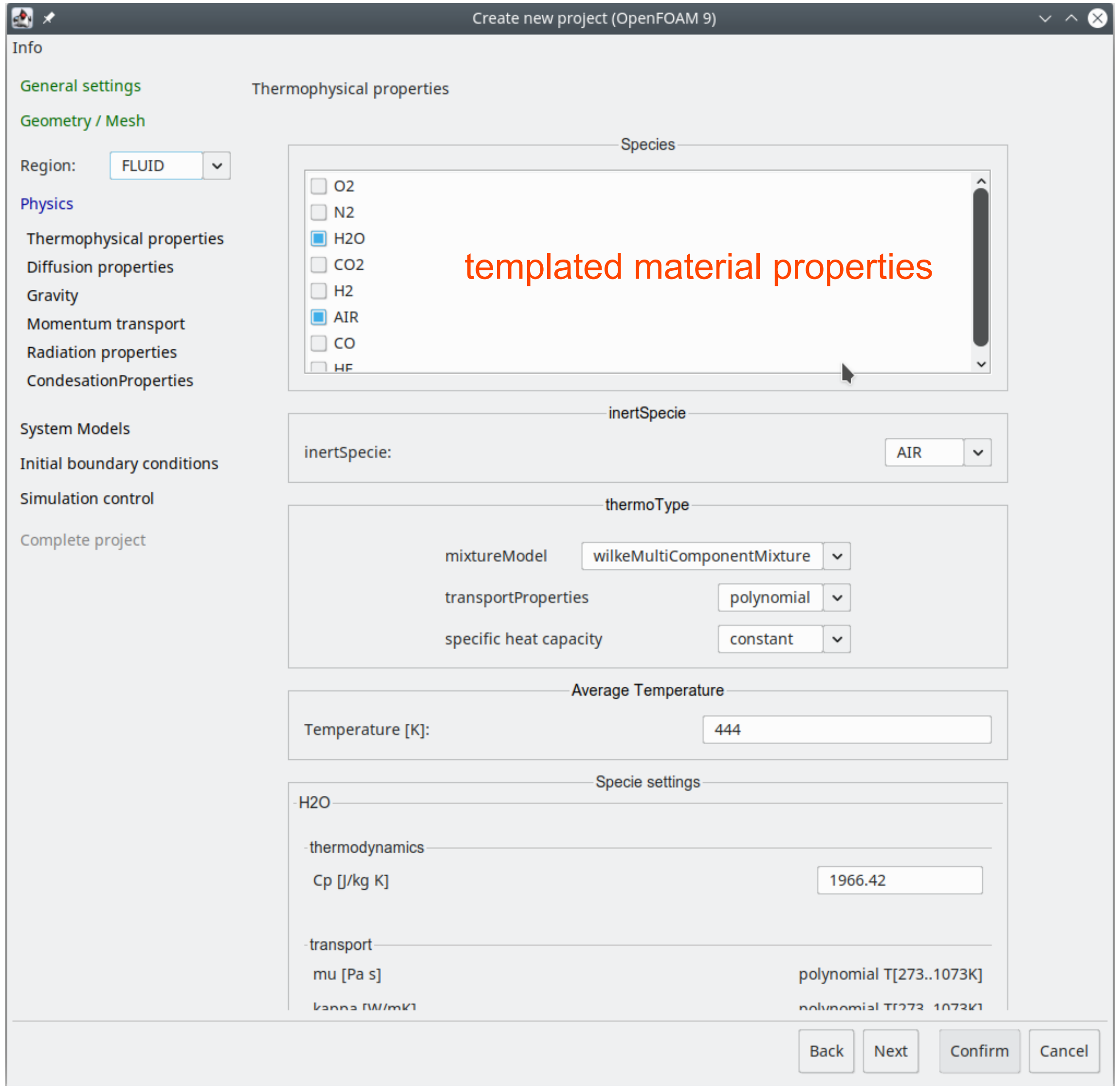
- Mesh import
  - Using OpenFOAM® utilities and libraries
  - Reads mesh quality metrics for further use (e.g. numerics settings)



CONTAINMENTFOAM FRAMEWORK

Guided Case Setup

- Mesh import
- Material properties of relevant species
  - Calculator
  - Polynomial fits (NIST data)



CONTAINMENTFOAM FRAMEWORK

JÜLICH Forschungszentrum

Guided Case Setup

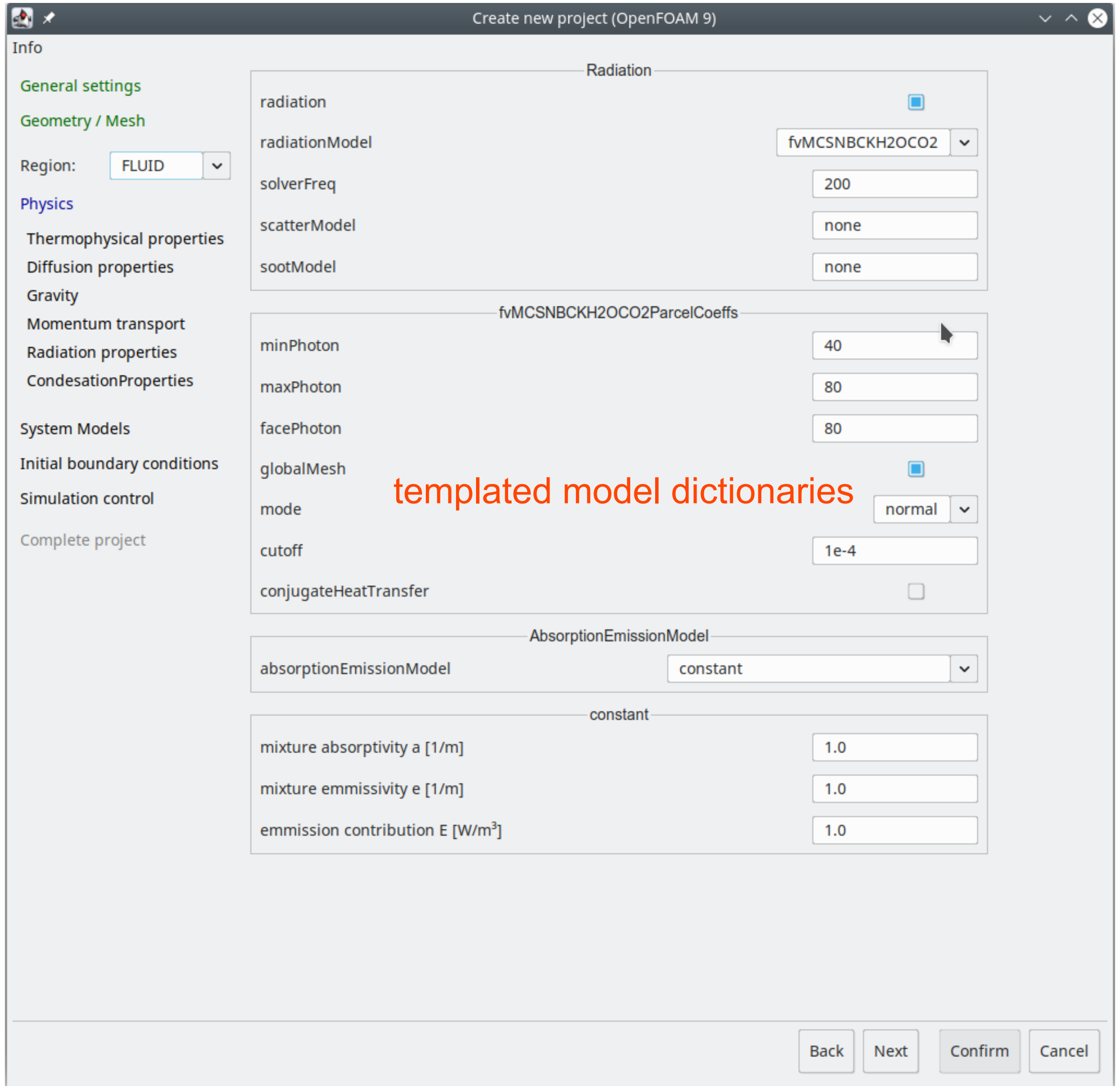
- Mesh import
- Material properties
- Model definition
  - Flexible extension by means of JSON-templates, logical rules and tooltips

```
"fvMCMParcelCoeffs":{
      "__settings__":["type=oneLineValue"],

      "__values__":
      [
      ["_show_{Label(text=minPhoton)}","_show_{TextField(text=4)};"],
      ["_show_{Label(text=maxPhoton)}","_show_{TextField(text=50)};"],
      ["_show_{Label(text=facePhoton)}","_show_{TextField(text=1)};"],
      ["_show_{Label(text=cutoff)}","_show_{TextField(text=1e-2)};"]
      ]
},

  "absorptionEmissionModel":{
      "__settings__":["type=oneLineValue"],

      "__values__":
      [
      ["_show_{Label(text=absorptionEmissionModel)}","_show_
      {ChoiceBox(text=[constantAbsorptionEmission,nongreyMeanAbsorptionEmission])};"]
      ]
  },
```

default parameters

model selection

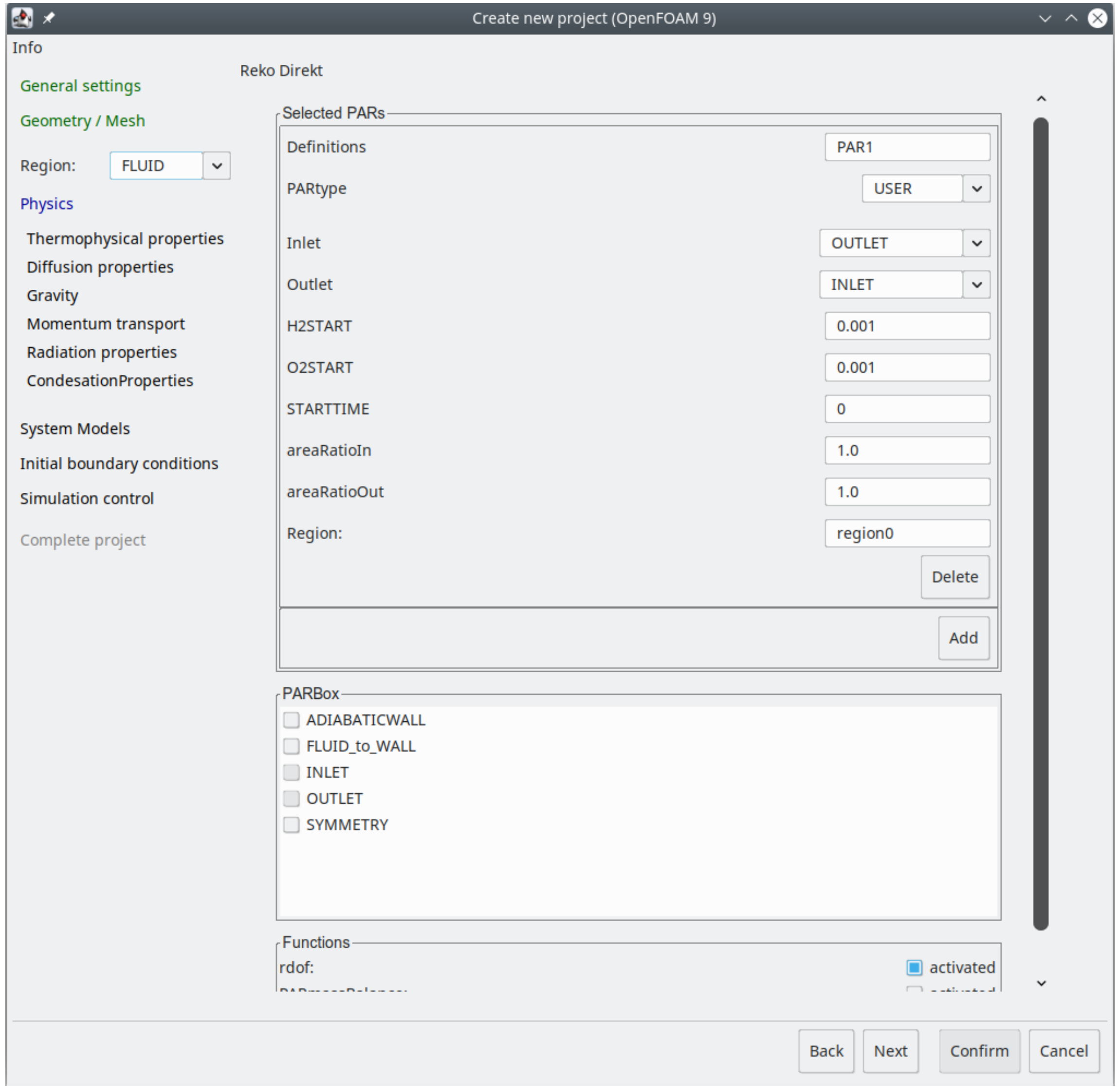
  - GUI workflow in analogy to OF case structure



CONTAINMENTFOAM FRAMEWORK

Guided Case Setup

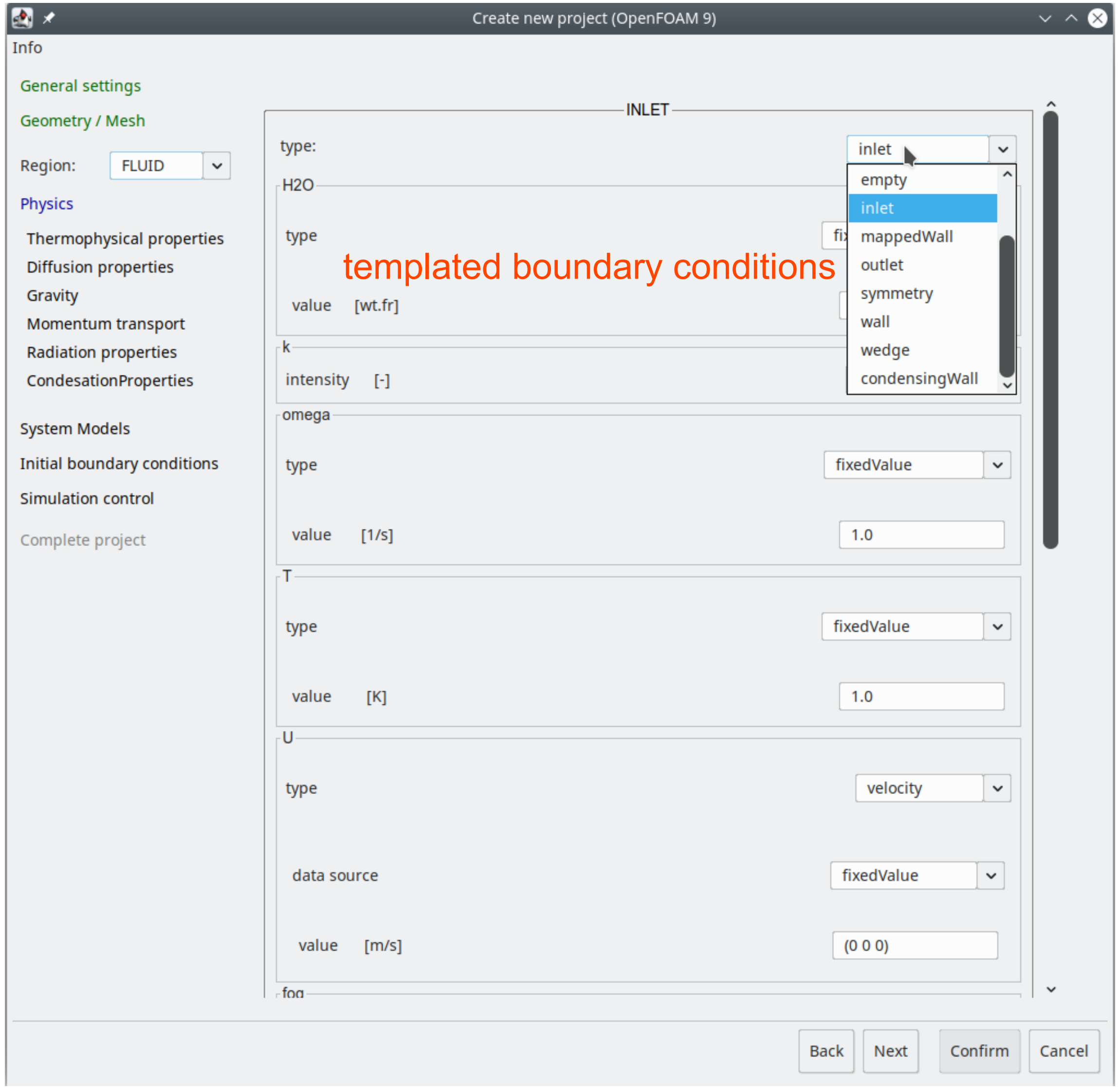
- Mesh import
- Material properties
- Model definition
- System models
  (mesh manipulation in background)



CONTAINMENTFOAM FRAMEWORK

Guided Case Setup

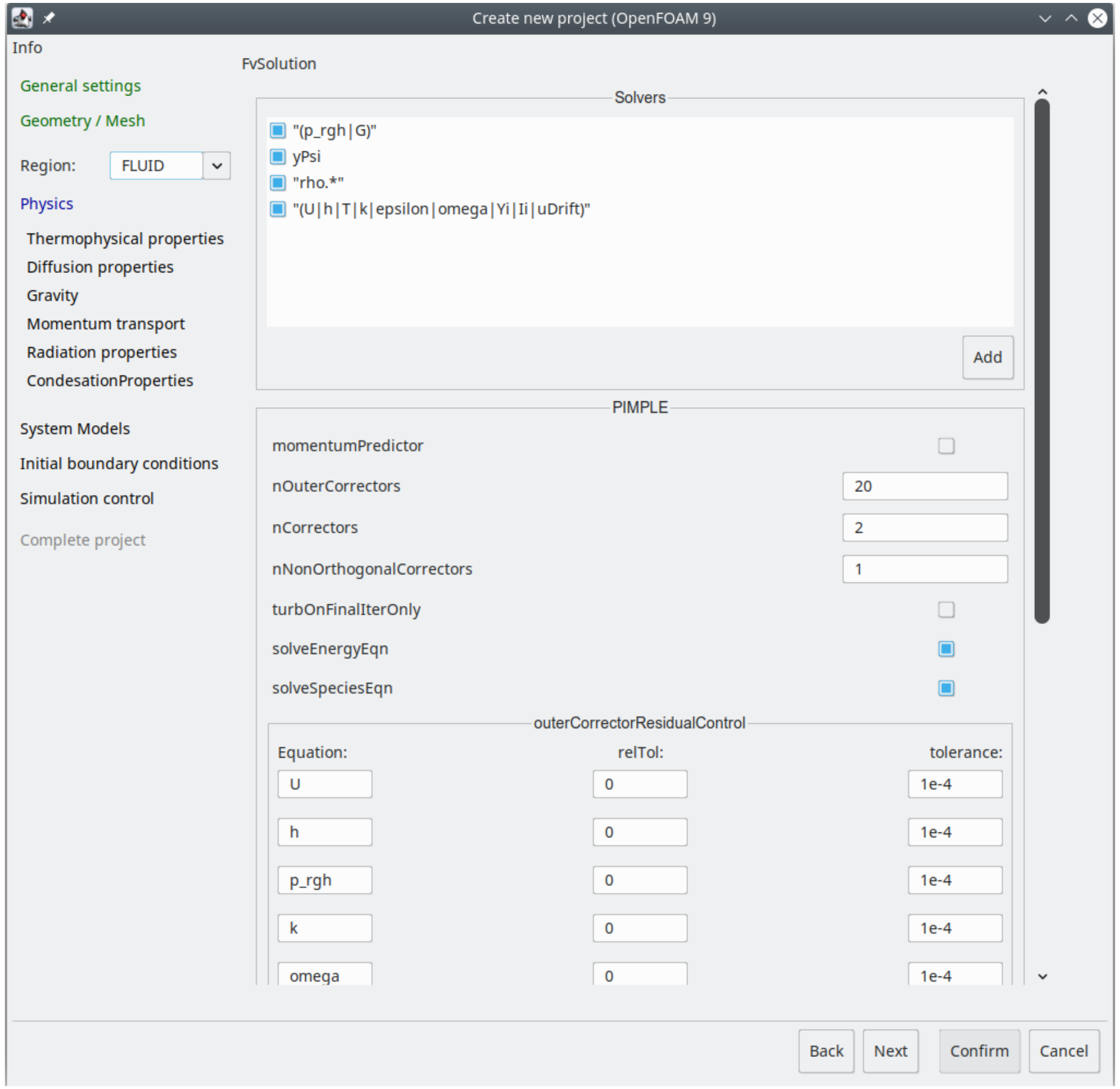
- Mesh import
- Material properties
- Model definition
- System models
- Consistent IC & BC specification
  - Predefined boundary types (‚condensing wall‘, ‚inlet‘ etc.)
  - csv import, table editor, global variables..



CONTAINMENTFOAM FRAMEWORK

Guided Case Setup

- Mesh import
- Material properties
- Model definition
- System models
- Consistent IC & BC specification
- Numerics and simulation control
  - Include predefined functionObjects (e.g. massBalance)
  - Best practice for numerical settings (fvSchemes and fvSolution)

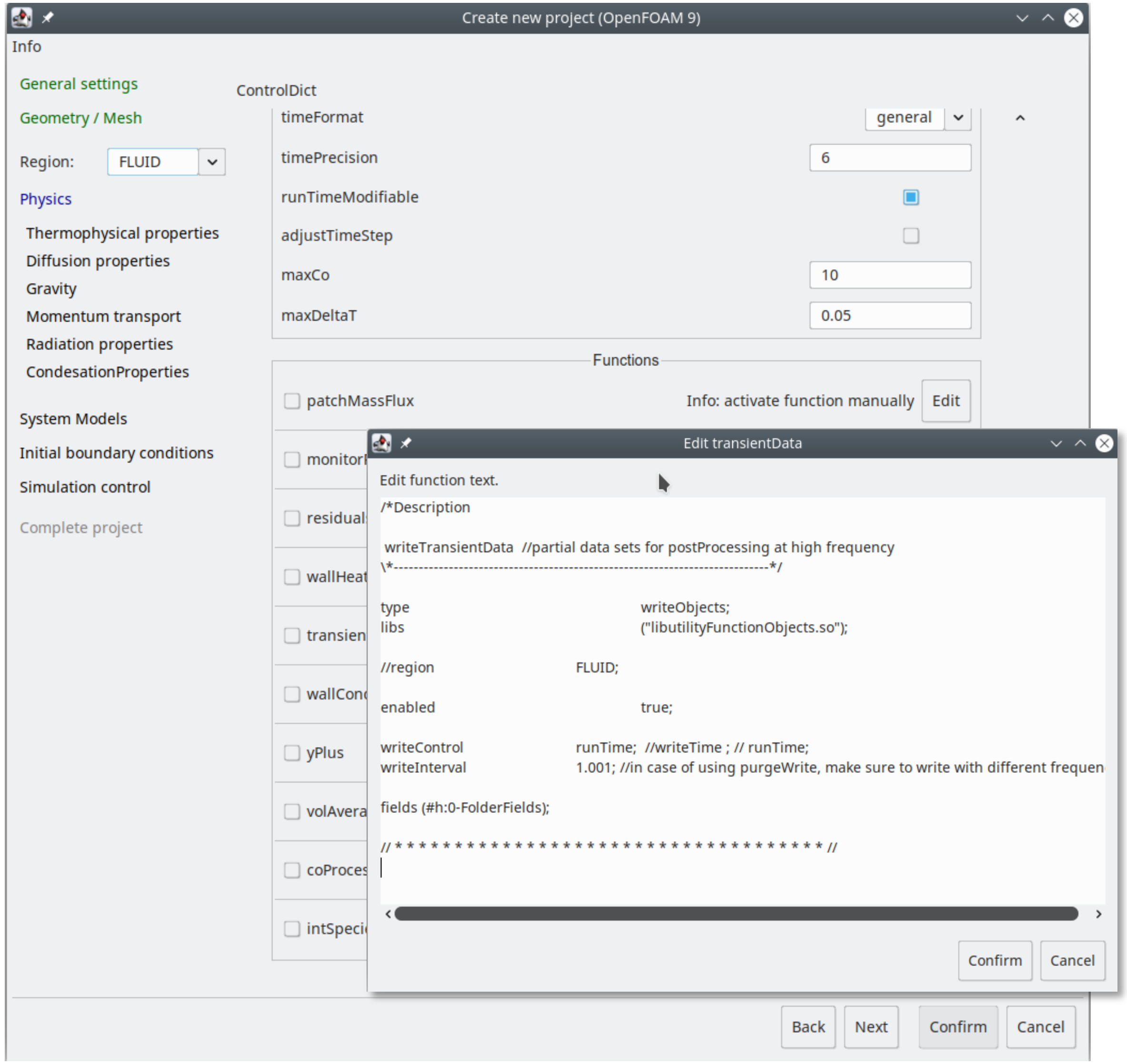


CONTAINMENTFOAM FRAMEWORK

Consistent, standardized Case Setup and Knowledge Preservation

- Mesh import
- Material properties
- Model definition
- System models
- Consistent IC & BC specification
- Numerics and simulation control
- Co/postprocessing (functionObjects)
- Further model integration ongoing

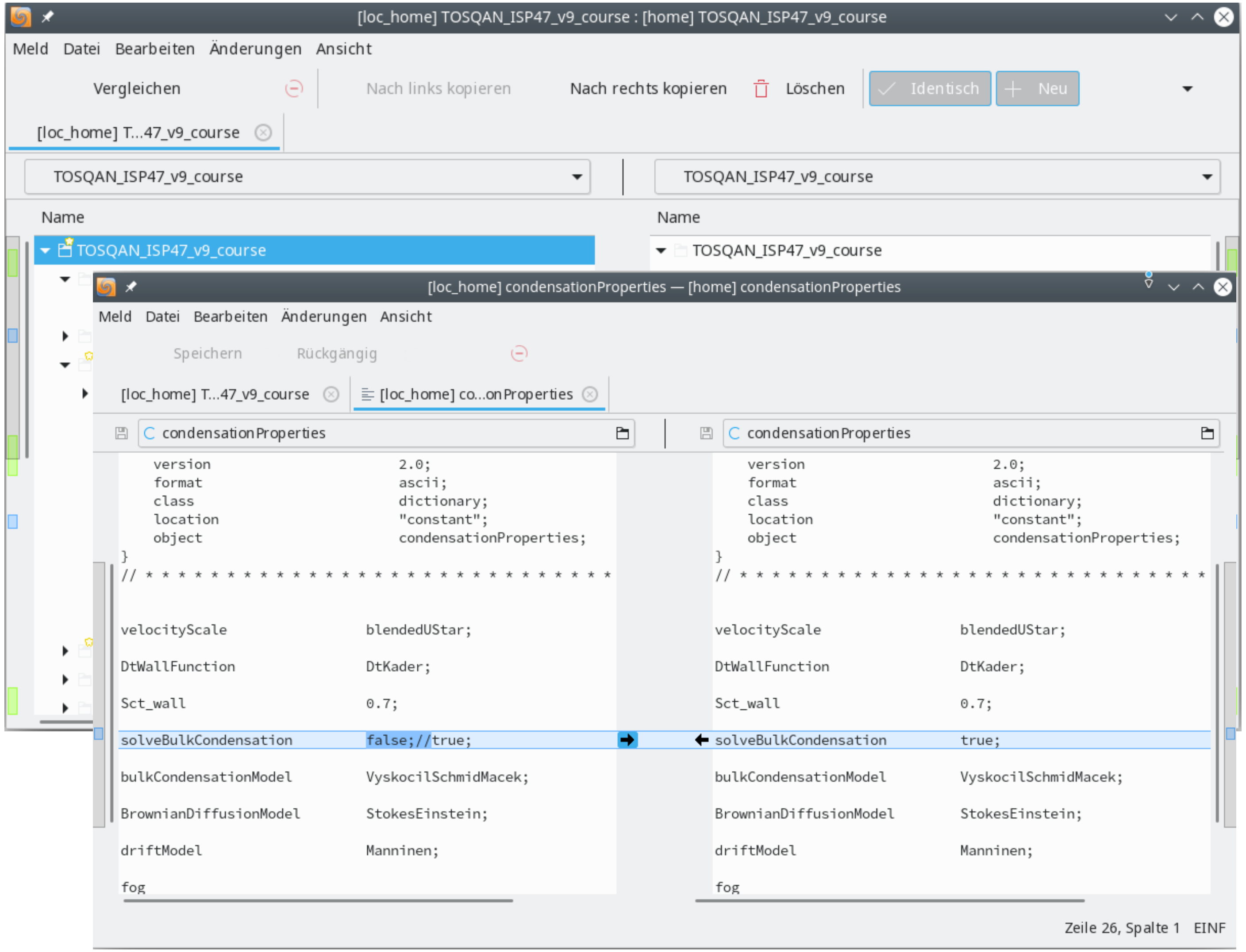
➢ Fast, reproducible and validated case setup is fundamental requirement for code use, trustworthy analysis and support



CONTAINMENTFOAM FRAMEWORK

Guided Case Setup – Concluding remarks

- The 'cfGUI' is intended to assist the user:
  - Understand 'cfGUI' as a kind of dynamic tutorial
  - Manual cloning and editing of existing cases is possible and a valid approach
  - To exploit full OF-functionality, manual edits are necessary (e.g. functionObjects)
  - Sometimes remaining syntax errors have to be resolved (version discrepancies with cF)
  - cfGUI aims to provide a starting point and fallback for case optimization
  - ➢ Keep a copy of the created case and use tools like meld-merge / git to track changes for debugging

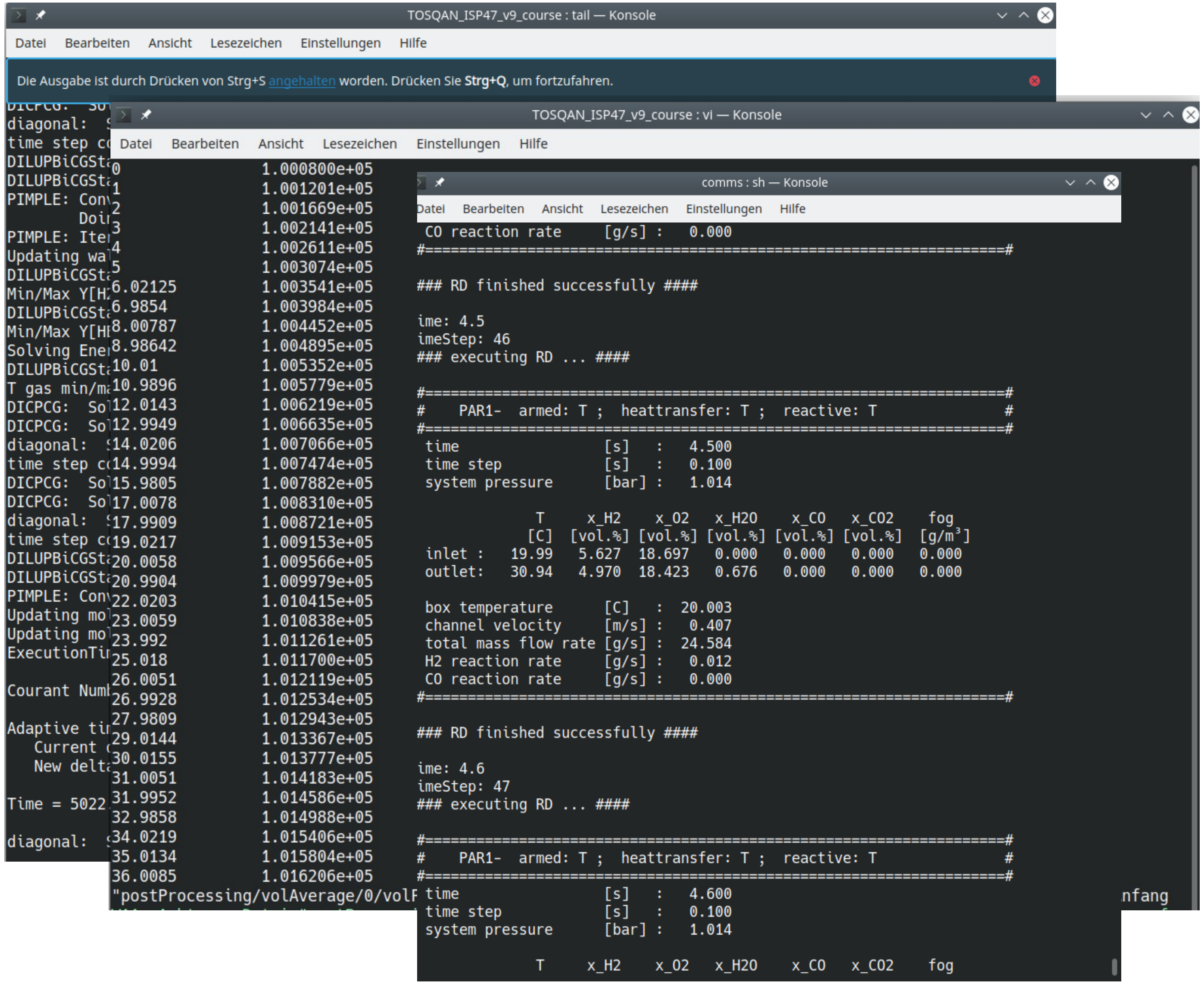


CONTAINMENTFOAM FRAMEWORK

Solution Monitor

- OpenFOAM provides relevant information at runtime,
  - Solver convergence and performance
  - functionObject output
  - coupled code logs
  - ..
- but:
  - trends are not visible
  - too much information
  - different formats
  - multiple windows ..

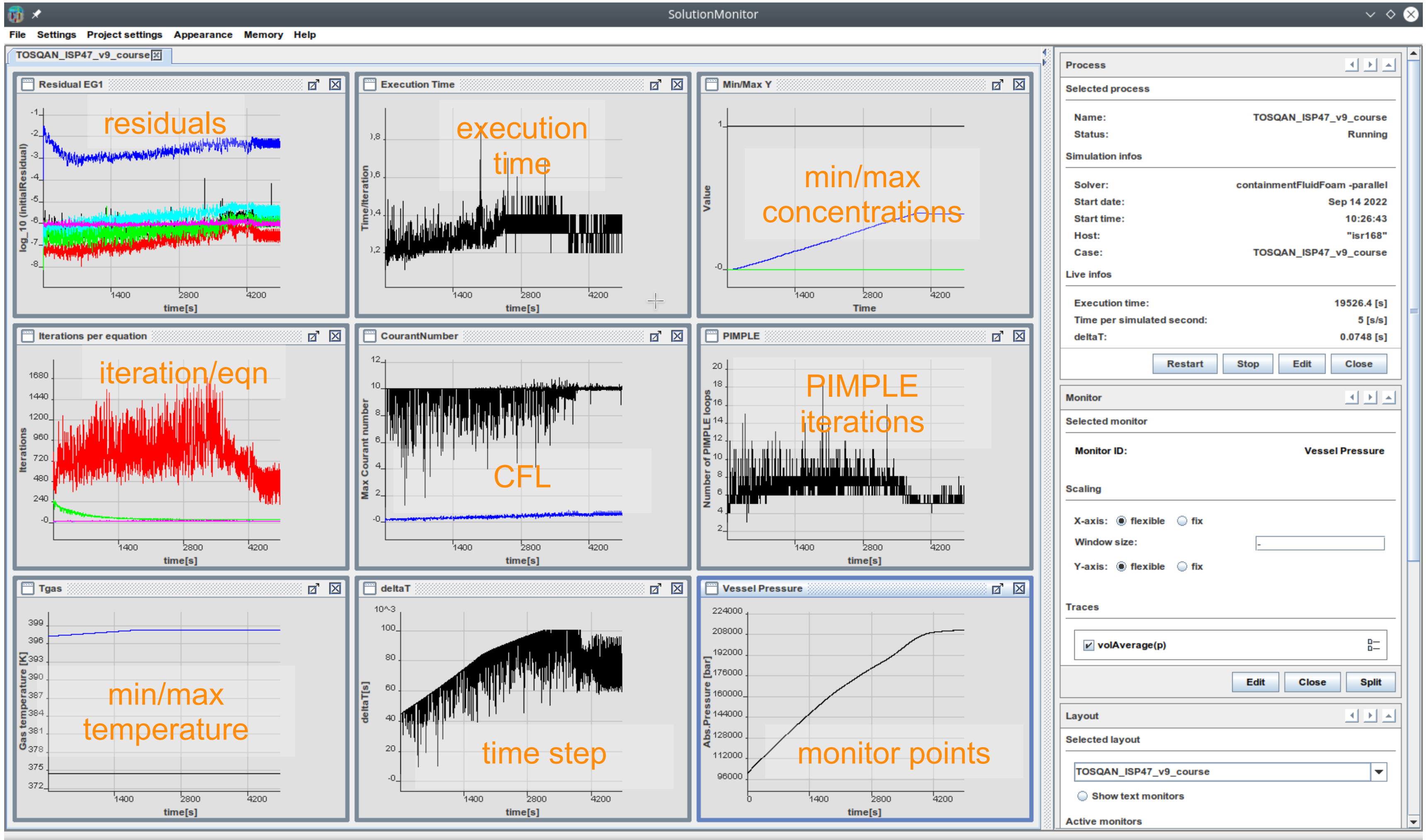
➢ Dedicated monitor for complex runs



CONTAINMENTFOAM FRAMEWORK

Solution Monitor

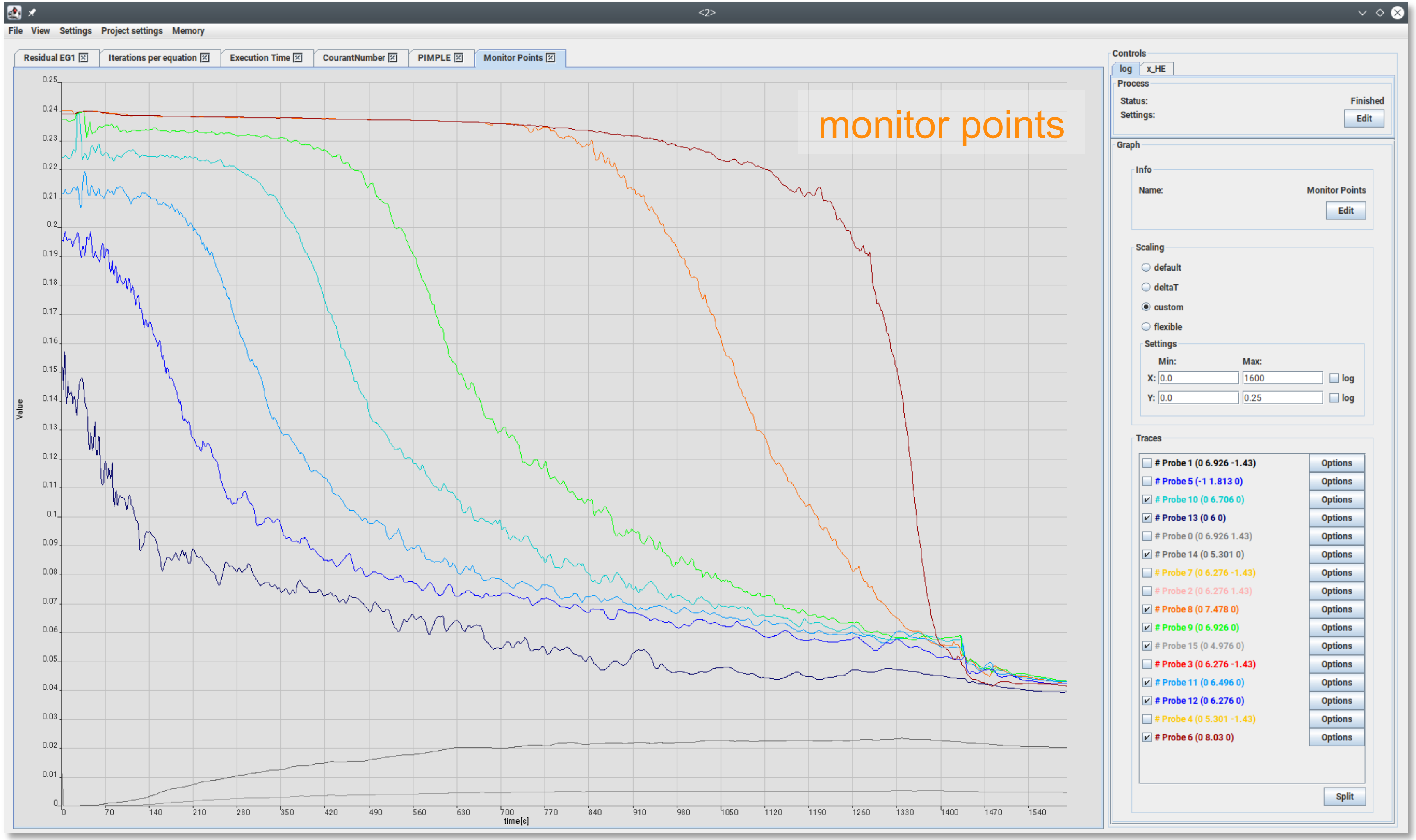
- Based on OpenJDK and jchart2D
  (http://jchart2d.sourceforge.net/)
  - Streams OpenFOAM logs, functionObject output and in principle any text log



CONTAINMENTFOAM FRAMEWORK

Solution Monitor

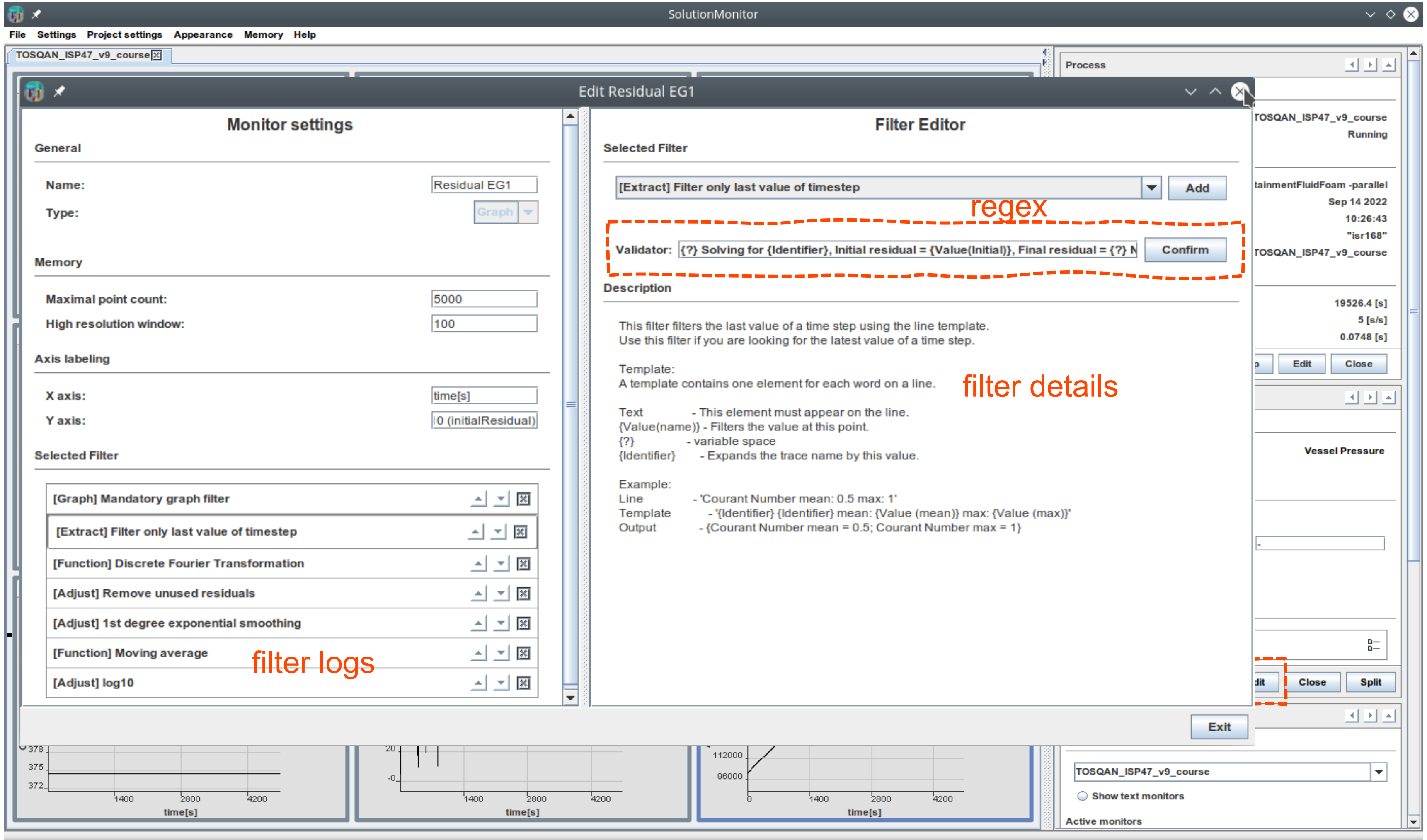
- Based on OpenJDK and jchart2D
  (http://jchart2d.sourceforge.net/)
  - Streams OpenFOAM logs and functionObject output
  - Tab and Grid view
  - Monitor multiple runs in parallel



CONTAINMENTFOAM FRAMEWORK

Solution Monitor

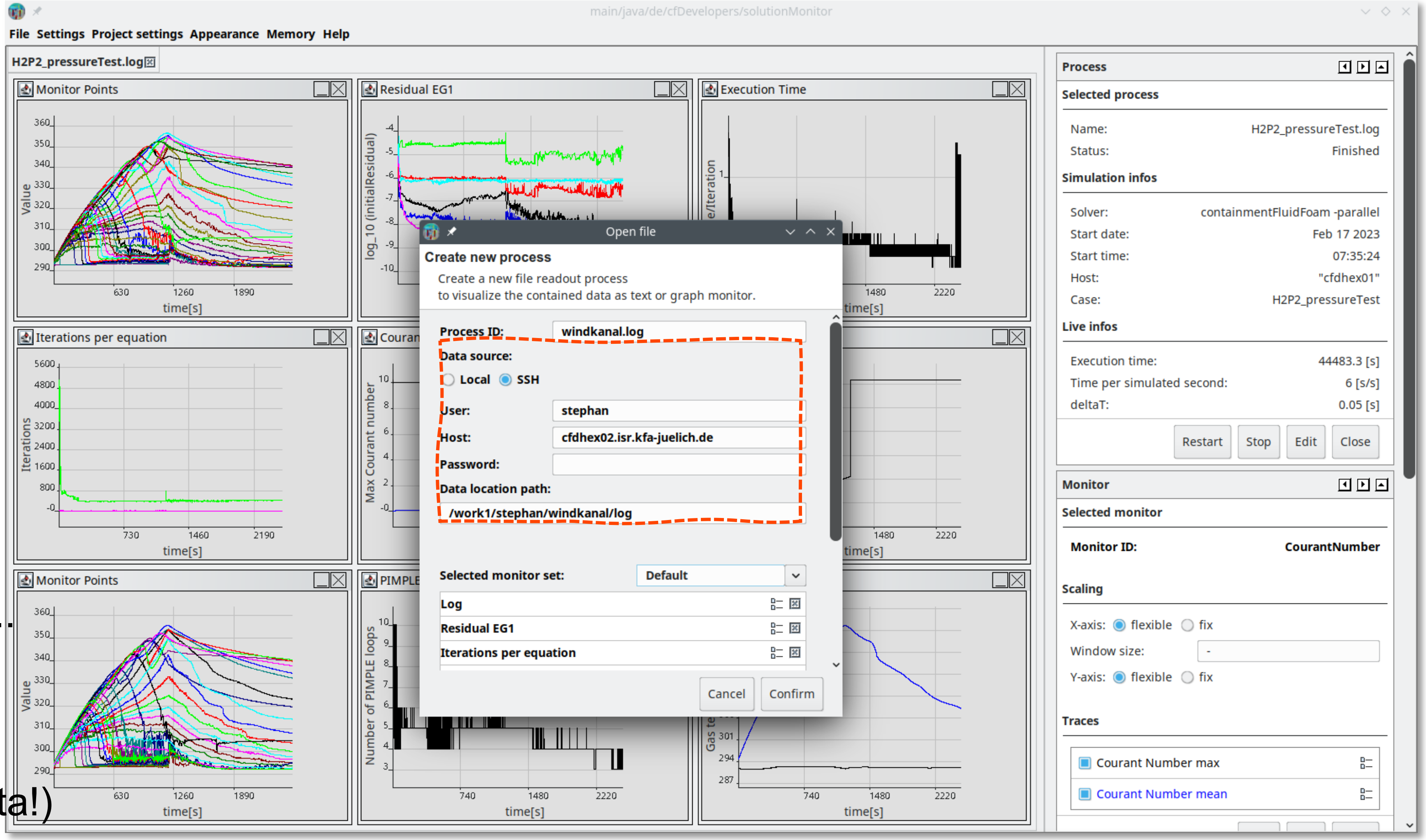
- Based on OpenJDK and jchart2D (http://jchart2d.sourceforge.net/)
  - Steams OpenFOAM logs and functionObject output
  - Tab and Grid view
  - Monitor multiple runs in parallel
  - Flexible RegEx syntax
  - Filters, e.g. moving average, exponential smoothing, FFT..
  - Save/load customized views (session files)



CONTAINMENTFOAM FRAMEWORK

Solution Monitor

- Based on OpenJDK and jchart2D (http://jchart2d.sourceforge.net/)
  - Steams OpenFOAM logs and functionObject output
  - Tab and Grid view
  - Monitor multiple runs in parallel
  - Flexible RegEx syntax
  - Filters, e.g. moving average, exponential smoothing, FFT…
  - Save/load customized views (session files)
  - remote monitoring (ssh – beta!)



OUTLINE

- Severe Accidents and Containment Analysis
- Development of containment∇FOAM
- Theoretical Background
  - Buoyancy driven turbulent multi-species flows
  - Condensation processes
  - Thermal radiation
  - System models (PARs, code coupling, burst discs, porous models)
- containment∇FOAM framework
  - repository
  - cfGUI and cfSolutionMonitor
- Summary and Conclusions

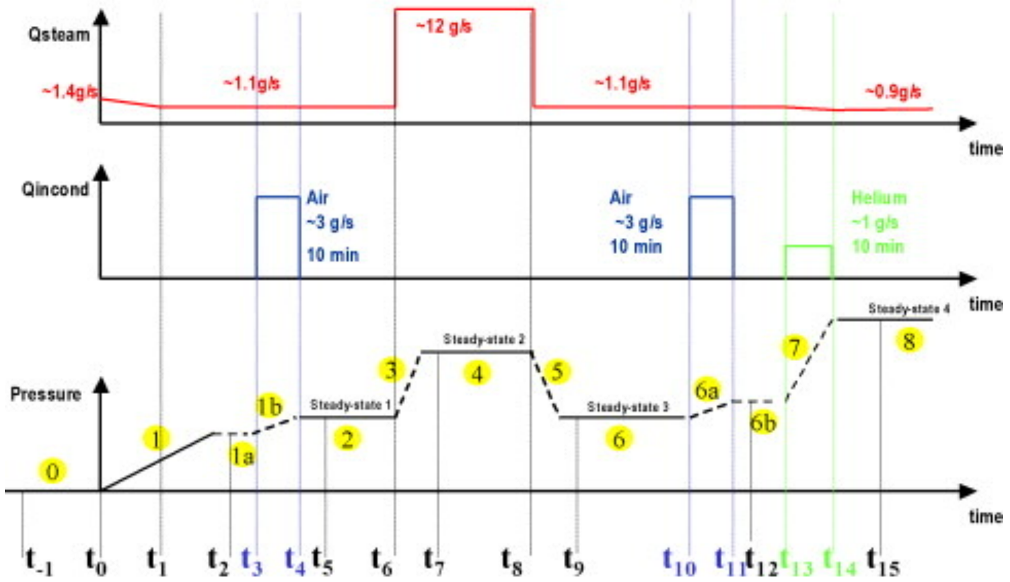
SUMMARY AND CONCLUSIONS

- containment∇FOAM is developed to analyze containment pressurization, flows, H_2/CO and aerosol behavior in dry PWR containments
  - Support experiments & transfer of experimental results to plant scale
  - Investigate interaction of physical phenomena and safety systems under representative conditions
  - Assess effectiveness of (passive) safety systems and measures
- tailored and well integrated model basis for expected containment conditions
  - Physical (CFD) models
  - Models for system feedback
- future work: revision and extension of model basis towards iPWR safety assessment
- summary of best practices and standard procedures provided as a starting point

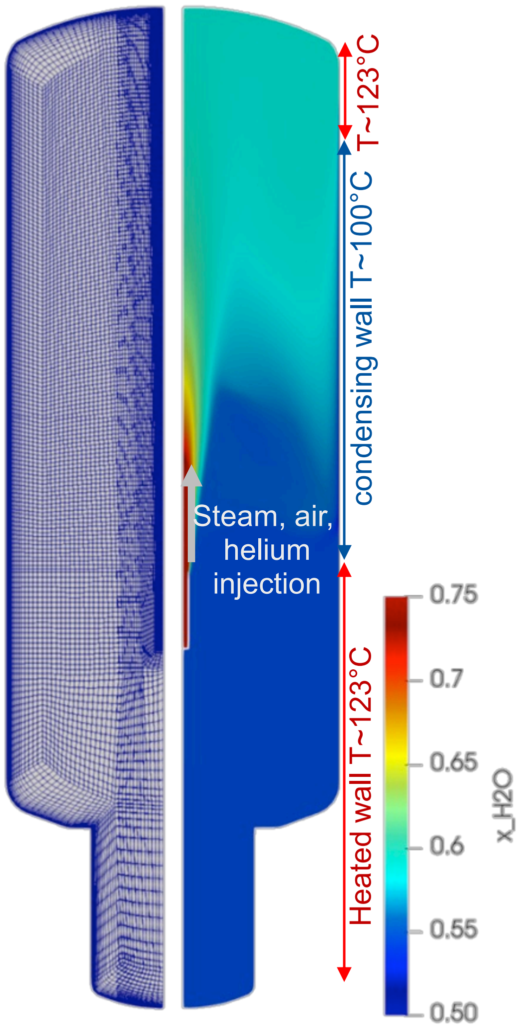
TRY YOURSELF - TOSQAN-ISP47

Introduction

- ISP-47 on containment thermal hydraulics - TOSQAN ($7m^3$) tests
  - Reference 🕮 Malet et al. NED(240), pp.3209–3220, 2010, https://doi.org/10.1016/j.nucengdes.2010.05.061
  - Aim: 'Separate effect tests' for wall condensation under different conditions to aid more complex analysis of MISTRA ($100m^3$) and THAI ($60m^3$) sequences
    - Series of transients and steady states:



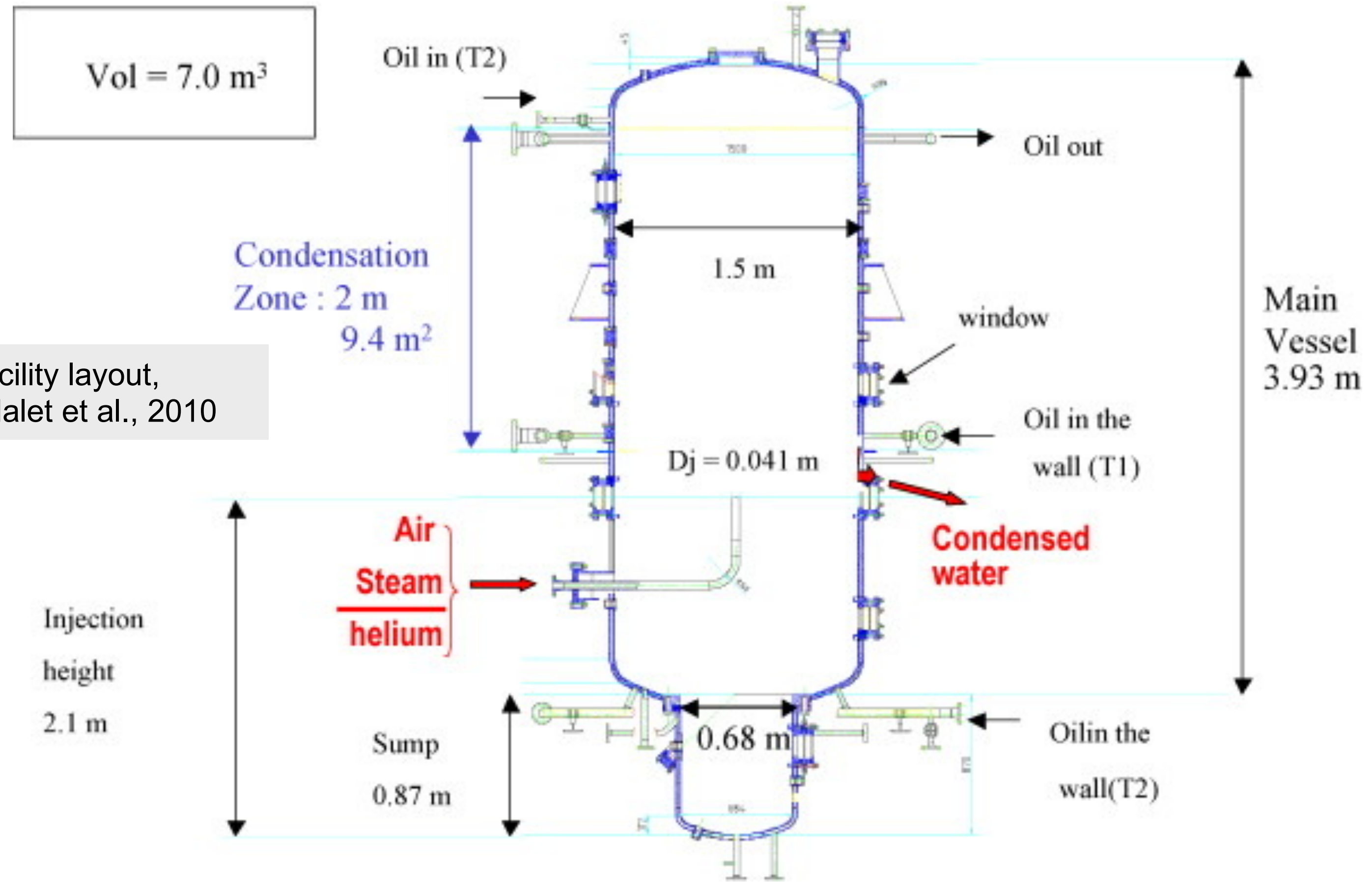
Test procedure,
from Malet et al., 2010



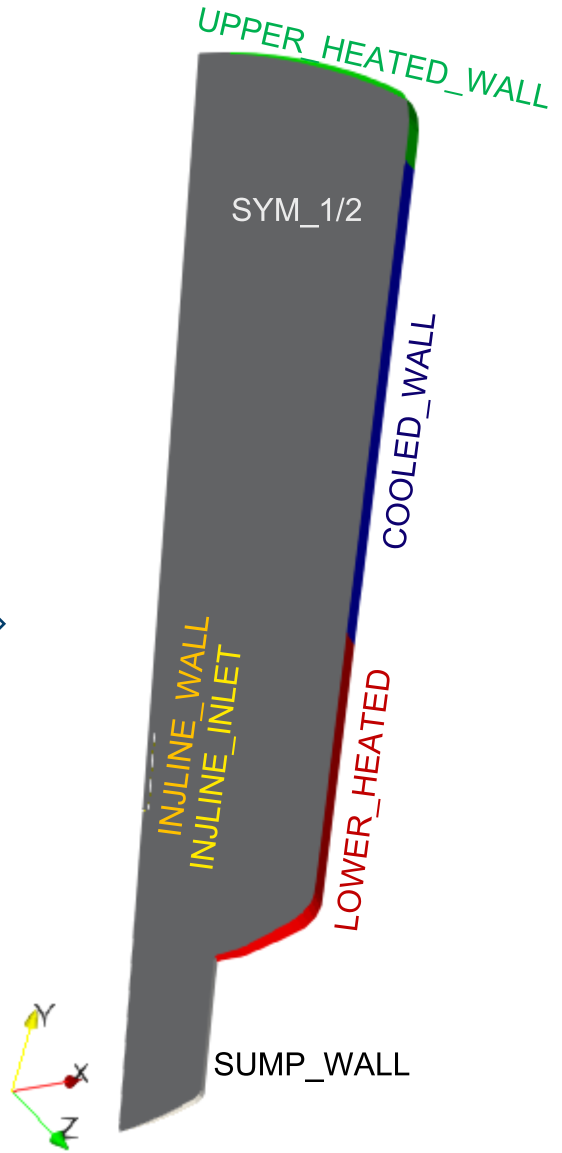
TRY YOURSELF - TOSQAN-ISP47

Geometry and Mesh

- 2D axis-symmetric model:



Facility layout,
from Malet et al., 2010

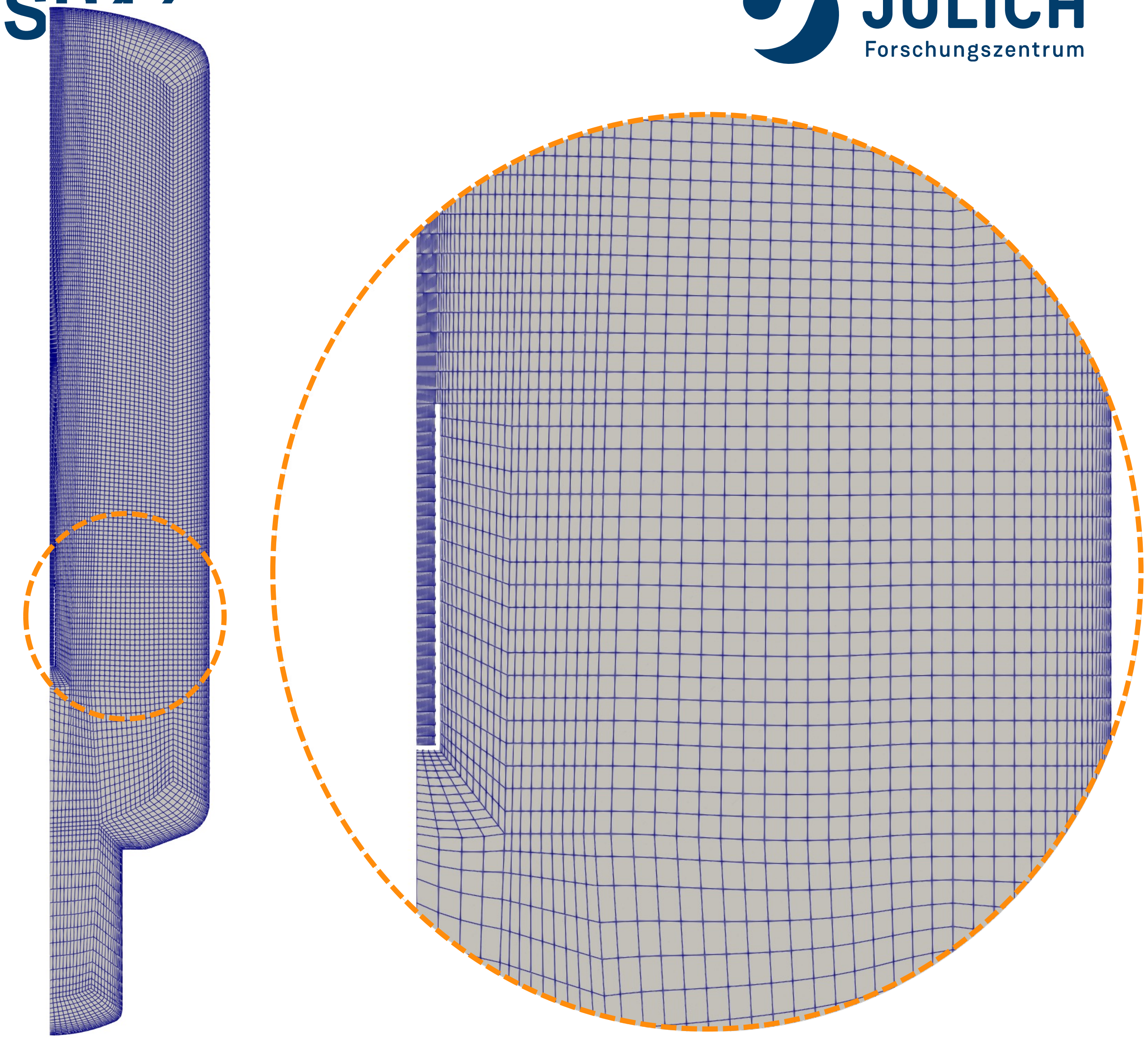


TRY YOURSELF - TOSQAN-IS

Geometry and Mesh

- 2D axissymmetry, 6 deg mesh slice:
  - ~13450 cells
  - checkMesh output:

```
Checking patch topology for multiply connected surfaces...
    Patch                  Faces    Points   Surface topology
    INNER_SUMP_WALL        30       61       ok (non-closed singly connected)
    INNER_LOWER_HEATED_WALL68       138      ok (non-closed singly connected)
    INNER_UPPER_HEATED_WALL62       125      ok (non-closed singly connected)
    INNER_COOLED_WALL      99       200      ok (non-closed singly connected)
    INJLINE_WALL           50       101      ok (non-closed singly connected)
    INJLINE_INLET          14       29       ok (non-closed singly connected)
    SYM_1                  13684    13963    ok (non-closed singly connected)
    SYM_2                  13684    13963    ok (non-closed singly connected)

Checking geometry...
    Overall domain bounding box (0 0 -0.039252) (0.748972 4.81549 0.039252)
    Mesh has 2 geometric (non-empty/wedge) directions (1 1 0)
    Mesh has 3 solution (non-empty) directions (1 1 1)
    Wedge SYM_1 with angle 3 degrees
    Wedge SYM_2 with angle 3 degrees
    All edges aligned with or perpendicular to non-empty directions.
    Boundary openness (-1.28547e-16 -2.84232e-19 5.1679e-15) OK.
    Max cell openness = 1.0891e-15 OK.
    Max aspect ratio = 69.5939 OK.
    Minimum face area = 1.12061e-07. Maximum face area = 0.00272496.  Face area magnitudes OK.
    Min volume = 7.13296e-10. Max volume = 4.80798e-05.  Total volume = 0.116843.  Cell volumes OK.
    Mesh non-orthogonality Max: 49.2529 average: 14.2296
    Non-orthogonality check OK.
    Face pyramids OK.
    Max skewness = 2.49629 OK.
    Coupled point location match (average 0) OK.

Mesh OK.
```



TRY YOURSELF - TOSQAN-ISP47

Initial and Boundary Conditions

- Available information:

Table 3
Wall temperature characteristics.

Stage	Description	Ref. time	Calculation times (s)	Mean condensing wall temperature (°C)	Mean upper non condensing wall temperature (°C)	Mean lower non condensing wall temperature (°C)
0	Initial phase	$t_{-1}-t_0$	−600 to 0	101.3 ± 1.0	122.0 ± 1.0	123.5 ± 1.0
1	T					
1 + 1a	T					
1b	T					
2	S					
3 + 4	T					
5–8	T					

Table 2
Injection characteristics (mass-flow rate and temperature).

Stage	Description	Ref. time	Calculation times (s)	Steam mean mass-flow rate (g/s)	Injection mean temperature (°C)	Air mean mass-flow rate (g/s)	Helium mean mass-flow rate (g/s)
0	Initial phase	$t_{-1}-t_0$	−600 to 0	–	–	–	–
1	Transient 1	t_0-t_1	0–1800	1.40–1.14, linear function of time	124 ± 3	–	–
1 + 1a	Transient 1 + short steady-state 1a	t_1-t_3	1800–5000	1.14 ± 0.05	125 ± 3		–
1b	Transient—air	t_3-t_4	5000–5600	1.14 ± 0.05	125 ± 3	3.16 ± 0.02	–
2	Steady-state 1	t_4-t_6	5600–6500	1.11 ± 0.10	126 ± 0	–	–
3 + 4	Transient 2 and steady-state 2	t_6-t_8	6500–9500	12.27 ± 0.12	132 ± 0	–	–
5	Transient 3	t_8-t_9	9500–12000	1.11 ± 0.11	131 ± 0	–	–
6	Steady-state 3	t_9-t_{10}	12000–13000	1.11 ± 0.06	126 ± 0		
6a	Transient—air					3.16 ± 0.02	–
6b	Short steady-state						
7	Transient 4					–	1.03 ± 0.02
8	Steady-state 4					–	–

Table 1
Initial conditions before steam injection (between t_{-1} and t_0, stage 0).

Absolute total pressure (bar)	1
Mean upper non condensing wall temperature (°C)	122.0
Mean lower non condensing wall temperature (°C)	123.5
Mean condensing wall temperature (°C)	101.3
Mean gas temperature (°C)	115.4
Air volume fraction (%)	100
Helium and steam volume fraction (%)	0

IC and BC,
from Malet et al., 2010

TRY YOURSELF - TOSQAN-ISP47

Initial and Boundary Conditions

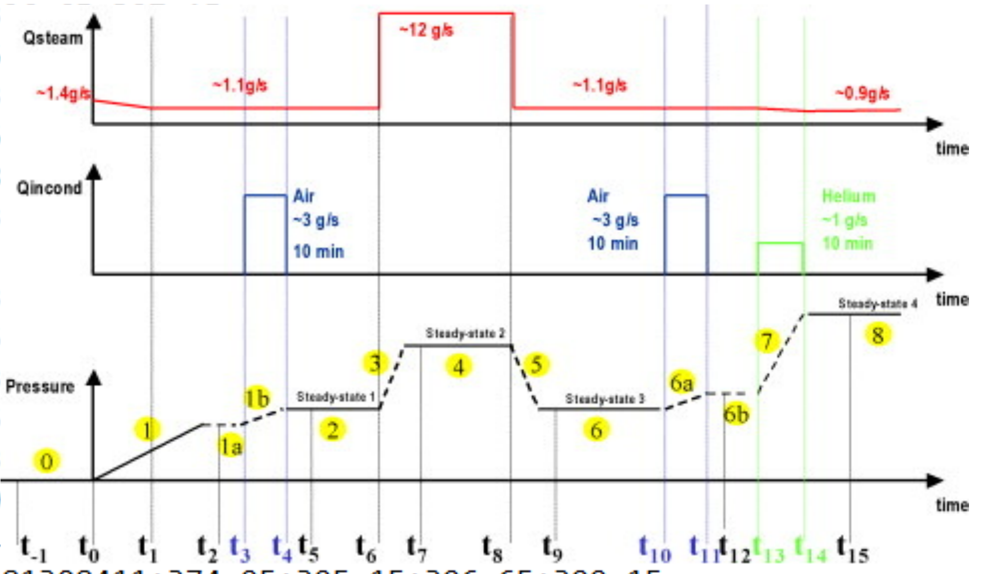
- Boundary conditions transformed into csv format:
  - SI units
  - mfr reduced for 6° slice
  - linear interpolation between time points (short intermediate times)

transientInp_6deg

transientInp_6deg - Editor

Datei Bearbeiten Format Ansicht Hilfe

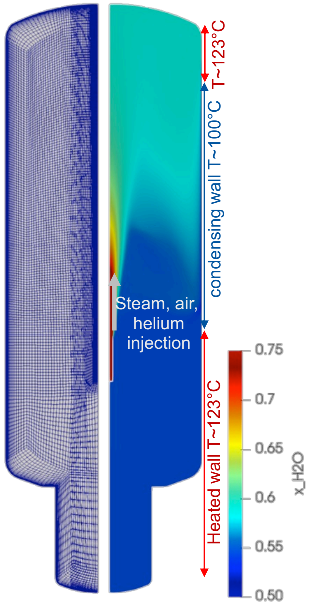
```
time[s];mtotal[kg/s];Ysteam;Yair;Yhelium;Tcooled[K];Tupperheated[K];TlowerHeated[K];Tinj[K]
0;0;1;0;0;374.45;395.15;396.65;397.15
0.1;2.33333E-05;1;0;0;374.45;395.15;3
1800;0.000019;1;0;0;374.45;395.15;396
1800.1;0.000019;1;0;0;374.45;395.15;3
5914;0.000019;1;0;0;374.45;395.15;396
5914.1;7.16667E-05;0.265116279;0.7348
6514;7.16667E-05;0.265116279;0.734883
6514.1;0.0000185;1;0;0;374.45;395.15;
11037;0.0000185;1;0;0;380.95;395.15;3
11037.1;0.0002045;1;0;0;380.95;395.15
18544;0.0002045;1;0;0;380.95;395.15;3
18544.1;0.0000185;1;0;0;374.95;395.15
23114;0.0000185;1;0;0;374.95;395.15;3
23114.1;7.11667E-05;0.259953162;0.740
23714;7.11667E-05;0.259953162;0.74004
23714.1;3.56667E-05;0.518691589;0;0.481308411;374.95;395.15;396.65;399.15
24314;3.56667E-05;0.518691589;0;0.481308411;374.95;395.15;396.65;399.15
24314.1;1.48333E-05;1;0;0;374.95;395.15;396.65;411.15
34000;1.48333E-05;1;0;0;374.95;395.15;396.65;411.15
```



HANDS-ON TOSQAN-ISP47

Running & postProcessing

- Postprocessing / evaluation:
  - Vessel pressure evolution
  - Mass balance
  - y^+ values



TOSQAN-ISP 47 scenario (l) and pressurization transient (r),