### **Retrospect, Status and Perspective of the Development** of containmentFOAM

<u>S. Kelm</u>, M. Kampili, G. Vijaya Kumar, X. Liu, A. George, R. Ji, L.M.F. Cammiade, K. Arul Prakash, H.-J. Allelein

IAEA Technical Meeting on the Development and Application of Open-Source Modelling and Simulation Tools for Nuclear Reactors, Politecnico di Milano, Italy, June 20-24<sup>th</sup> 2022



Supported by:



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

based on a decision of the German Bundestag Project No. 150 1633B



### OUTLINE

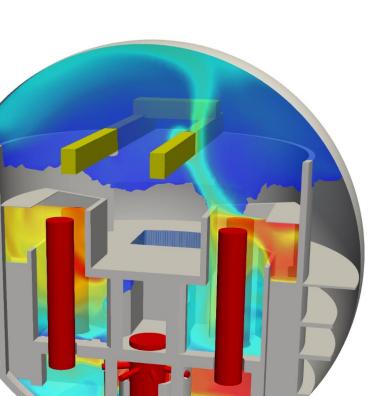
- Introduction
  - Background and Motivation
  - Strategy and General Considerations
  - Status of containment  $\nabla F \widehat{m} AM$
- Open-source challenges
  - Maintenance, distribution
  - User-Developer interaction
- Best practices
- Summary and Perspective



### BACKGROUND

- Development of containment VF AM [1] as an open basis to analyze containment pressurization, flows, H<sub>2</sub>/CO and aerosol behavior:
  - Basis for our research within the Helmholtz Nusafe program:
    - Replacement of previous commercial code basis & legacy code
    - 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
    - Contribution to national CFD reference package for NRS
  - Carrier to disseminate our research and ensure its application
  - International cooperation (e.g. IITM, IAEA-ONCORE, OECD/NEA)
  - Attractive platform for education, training and maintenance of competence 0.1





J. Stev

steam (vol.fr)



## **CONTAINMENTFOAM ENVIRONMENT**



### Active developers team

PI

(permanent)





PhD students

students & trainees

technical staff (permanent)



former PhD students

- > Mostly temporary contributors with different levels of qualification!
- Current collaborators, users & beta-testers:

PostDoc



## **MOTIVATION TO USE THE OS APPROACH**

Obviously:

- FAIR is the way to do meaningful publicly funded research!
- Many further benefits:
  - Visibility of the individual's work and the project:

> Motivation for contributors and new applicants to join

- Reusability of the research output by others:
  - Increases impact and KPI (citations)
  - In-line with Helmholtz digitalization strategy
- Involvement of temporary staff at different education levels:
  - Possibility to keep them involved beyond their contract
- International collaboration:
  - > No troubles with license agreements but maybe contributors agreements needed





#### IEK-14 Safety Research | S. Kelm et al. IAEA ONCORE TM, Politecnico di Milano, Italy, June 20-24<sup>th</sup> 2022

## **DEVELOPMENT OF CONTAINMENTFOAM**

#### **Strategy and General Considerations**

- Coordinated R&D effort (currently 14 active contributors, cumulative > 25 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
    - o 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





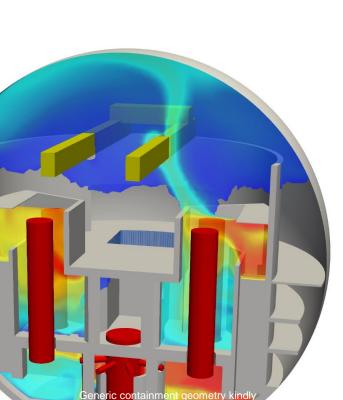
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# **STATUS OF CONTAINMENTFOAM**

Modeling Pressurization, Aerosol Transport and H<sub>2</sub>/CO Gas Mixing and Mitigation

- Flows and Transport Phenomena
  - Efficient Multi-Species Solver: effective binary diffusion; Wilke mixture (
  - **Turbulence transport**: k- $\omega$  SST model with buoyancy terms, simple and generalized gradient diffusion hypothesis formulation
  - Conjugate heat transfer
  - Wall condensation: single phase diffusion layer model, implemented as face fluxes ( ) dedicated wall treatment
  - Fog formation: drift flux model with PBM (, two phase formulation (
  - o Gas radiation: Emission-based Reciprocity Monte Carlo Method, ( SNBCK and LBL spectral models (
  - Aerosol transport: LPT with Continuous Random Walk model for turbulent dispersion, 🧭 Eulerian drift flux model including hygroscopic growth
- Technical Systems and Components
  - PARs: Code coupling with mechanistic model REKODIREKT
  - Burst discs, flaps, doors: conditional mesh interfaces

• Heat exchangers: porous media ( Fluids (2021) 6, no. 3: 100. https://doi.org/10.3390/fluids6030100



steam (vol.fr)

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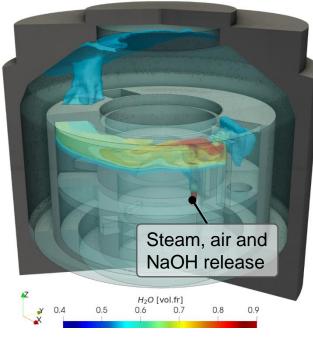
# **STATUS OF CONTAINMENTFOAM**



**Applications** 

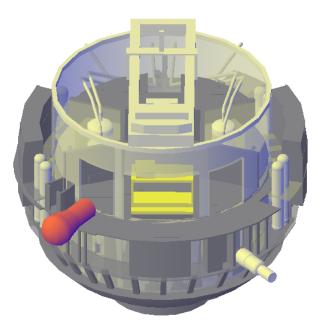
#### **ISP-37 VANAM M3**

- thermo-fluid dynamics and aerosol distribution



- 600 m<sup>3</sup>, 20.000 s
- ~ 400 ..1100 s / day @ 128 CPU

- German KONVOI PWR (1400 MW<sub>el</sub>)
  - flammable gas distribution, combustion risk and mitigation





POLITÉCN

DA( ICA

- Work-in-Progress (CAD model by UPM)
- ~ 70000 m<sup>3</sup>, *O* ~ 1000 s
- 💷 S. Kelm et al., "Technical Scale CFD Analysis of the Pressurization and Transport Processes in the Battelle Model Containment during the ISP 37 VANAM M3 Test ", accepted for publication at NUTHOS 13, Taichung, Taiwan, September 5-10, 2022
- L. S. Lopez et al., Development of a detailed 3D CAD model of a generic PWR-KWU containment as a basis for a better assessment of H2/CO combustion risk, Proc. ENYGF'21

### OUTLINE

- Introduction
  - Background and Motivation
  - Strategy and General Considerations
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- Open-source challenges
  - Maintenance, distribution
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- Best practices
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- Licensing: derived from the original code basis
  OpenFOAM
  The OpenFOAM Foundation
  GNU public license v 3.0
- Distribution: via gitlab <u>https://go.fzj.de/containmentFOAM</u>
  - Branching model: feature a open access ¦ restricted access merge + Wiki, issues ... (internal) release productive develop feature b mirror merge merge (internal) (public) (internal) (internal) merge feature c (internal)
- Iong-term maintenance (supported by BMUV, Project No. 150 1633B in collaboration with GRS, Project No. RS1603A)
  - mostly a 'non-scientific' work (implications on funding or visible research output)
  - but requires skilled scientists who know the models and their numerical implementation peculiarities
  - comprehensive efforts to follow refactoring of of the original code basis (OpenFOAM)



**Developer - User Interaction** 

- Challenges:
  - Derivation from / add-on to a famous OS-CFD package enables a broad distribution and usage
    - $\circ$  Known and unknown users  $\rightarrow$  different channels for communication
    - Users with different applications, background and experience (e.g., meshing, CFD, OpenFOAM, containment phenomenology & modeling etc.)
      - Skilled OpenFOAM users may have different established, but 'incompatible' workflows, modeling approaches etc.
      - Different applications may exceed the models' validity range targeted by the developers
      - How to prevent user errors (inconsistent setups, misunderstanding)
  - Specific developments are highly complex (product of 4 years PhD projects)
    - How to enable best 'usability' of new developments to provide user feedback to the developers ?
    - How to transfer the developers experience to the user?
  - Provide and maintain a useful documentation and user guidance
    - Successful usage is important to keep the user's group active
    - Limit time for support



#### **Developer - User Interaction**

- GitLab platform at FZJ -
  - Version management
  - CI/CD Environment
  - Ticket system
  - Wiki (only internal)
  - flexible account management via ,github accounts'

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#### **Developer - User Interaction**

- GitLab platform at FZJ
  - Version management
  - CI/CD Environment
  - Ticket system
  - Wiki
  - flexible account management
  - GitLab flavored Markdown files
     Model details

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Project overview	master ~ containmentfoam	doc / THEORY.md	Finde Datei Blame History Permalink
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Vergleichen	containmentFOAM is a multi-species and r processes inside confined domains e.g., a safety assessment. It contains submodels		at and mass transfer in buoyant flows, gas radiation heat transport, combustible gas
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Packages & Registries	Turbulence Modeling	Species equation	
🕛 Analysen	Wall Condensation	$rac{\partial\left( ho Y_{k} ight)}{\partial t}+ abla\cdot abla\cdot$	$( hoec{U}Y_k)=- abla\cdotec{J}_k+S_{Y_k}$
🖞 Wiki	Bulk Condensation and Fog Transport	where $\vec{J}_k$ is the diffusive mass flux and $S_{Y_k}$ is volumetric source term (= 0 Fick's law of diffusion	) unless explicitly defined) of the $k^{\rm th}$ specie. The diffusive mass flux $\vec{J}_k$ is described by
	Thermal Radiation Heat Transfer	$ec{J}_k$ =	$= - ho D_{k, ext{eff}}  abla Y_k$
🔏 Codeausschnitte	Aerosol Transport	in $\textit{containmentFOAM},$ the Soret effect or thermal diffusion flux $D_{k,T} \frac{\nabla T}{T}$ is	neglected.
🏝 Mitglieder	System Models:	Momentum equation	
🏟 Finstellungen	Passive Auto-Catalytic Recombiners	${\partial \left(  ho ec U  ight) \over \partial t} +  abla \cdot \left(  ho ec U \otimes  ight)  ight)$	$ec{U} \Big) = -  abla p +  abla \cdot  au +  ho ec{g} + ec{S}_{ ext{mom}}$
K Seitenleiste einklappen	Burst Discs / Doors	where $p$ is the pressure, $\vec{g}$ is the acceleration due to gravity, and $\vec{S}_{\rm mom}$ is the viscous stress tensor $\tau$ is defined as	he volumetric source term for the momentum equation ( $ec{S}_{ m mom}=$ 0, unless specified).
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#### **Developer - User Interaction**

- GitLab platform at FZJ •
  - Version management
  - CI/CD Environment
  - Ticket system
  - Wiki
  - flexible account management
  - GitLab flavored Markdown files
    - Model details
    - Recommended usage
    - Link to source files
    - References

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🕻 Codeausschnitte	Aerosol Transport	References								
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🗘 Finstellungen	Passive Auto-Catalytic Recombiners	2. B.A. Kader, "Tempe	erature and Concentration Profiles in	Fully Turbulent Boundary Lay	vers", International Jou	urnal of Heat and I	Mass Transf	fer 1981, 24(9) 🔁		
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		4. D.B. Spalding, A Si	ngle Formula for the Law of the Wal	Tokyo November 2-7, 2003 2 4. D.B. Spalding, A Single Formula for the Law of the Wall, Journal of Applied Mechanics 1961, 28, pp. 455-458						

foam-for-nuclear

 Quick links 
 FAQ A Board index

Source code / programming / AP

re-processing and mesh

Post-processing in Open

Miscellanea

GeN-Foam Subforums: Compiling,

OFFBEAT

Subforums: Con containmentFOAM

Subforums, FrCompline

and Documentation.

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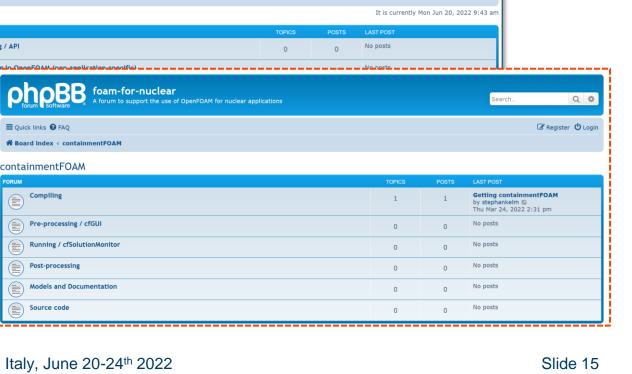
to support the use of OpenEOAM for nuclear applicat

### **UNIQUE OPEN SOURCE ISSUES**

**Developer - User Interaction** 

- Communication channels:
  - chat system (upon request / invitation) Mattermost
  - Discussion forum
    - https://foam-for-nuclear.org/phpBB/ thanks to Carlo Fiorina for hosting it !
  - <u>containmentfoam@fz-juelich.de</u>

> User support is mandatory, as the projects success depends on the number of users!



Search...

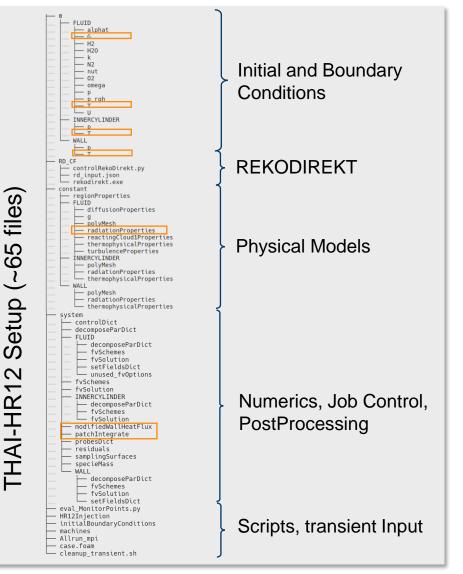


Q 🌣

🕼 Register 🙂 Login

**Developer - User Interaction** 

- Containment analysis comprises interaction of multiple physical phenomena and safety systems:
  - Definition in separate files (,dictionary')
  - Dependencies among dictionaries (and models)
  - Inconsistent definitions possible, which may not cause a crash
  - Broad variety of numerical methods and schemes
- >,Standard' & Best Practice required:
  - Prevent input errors
  - Ensure consistent model application
  - Enable comparable and reproducible analysis
  - Support / bug identification and fixing.





Definition ,gas radiation







- General idea:
  - Workflow, structure and syntax close to OpenFOAM
  - limit functionality to baseline model and fundamental functions
  - Enable easy entry for new users (only a mesh is needed)
  - Enable fallback for bug tracking
- Mesh import
  - Using OpenFOAM<sup>®</sup> utilities and libraries
  - Reads mesh quality metrics for further use (e.g. numerics settings)

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### **Developer - User Interaction**

- Mesh import
- Templated material properties
  - Calculator
  - Polynomial fits (NIST data)

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OpenJDK 🥂

#### **Developer - User Interaction**

- Mesh import
- Templated material properties
- Flexible model templates based on JSON, logical rules and tooltips by the containmentFOAM developers (no Java skills needed)

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OpenIDK 🕅

**A** 

### **Developer - User Interaction**

- Mesh import
- Templated material properties
- Flexible extension
- Consistent IC & BC specification
  - Predefined boundary types (,condensing wall', ,inlet' etc.)
  - csv import, table editor, global variables..

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Create new project (OpenFOAM



#### **Developer - User Interaction**

- Mesh import
- Templated material properties
- Flexible extension
- Consistent IC & BC specification
- Numerics and simulation control
  - Best practice for numerical settings (fvSchemes and fvSolution)

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IAEA ONCORE TM, Politecnico di Milano, Italy, June 20-24<sup>th</sup> 2022

### **Developer - User Interaction**

- Mesh import
- Templated material properties
- Flexible extension

IEK-14 Safety Research | S. Kelm et al.

- Consistent IC & BC specification
- Numerics and simulation control
  - Best practice for numerical settings (fvSchemes and fvSolution)
  - Include predefined functionObjects (e.g. mass/energy Balance)
- Fast, reproducible and verified case setup is fundamental requirement for code use, support and trustful analysis

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OpenIDK 🍂

#### Residual EG1 d' 🛛 Execution Time Solution Monitoring! execution time residuals

Iterations per equation

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780.

🗂 Tgas

matrix solver

iterations

min/max temp

14700

Page 1

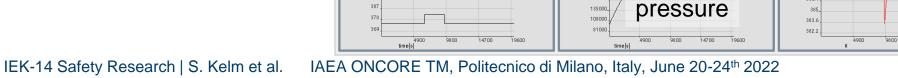
File Settings Project settings Memory Heli

Based on OpenJDK X and jchart2D (http://jchart2d.sourceforge.net/)

Good setup an then ?

**Solution Monitor** 

- Streams OpenFOAM logs and functionObject output
- Grid and tabbed view



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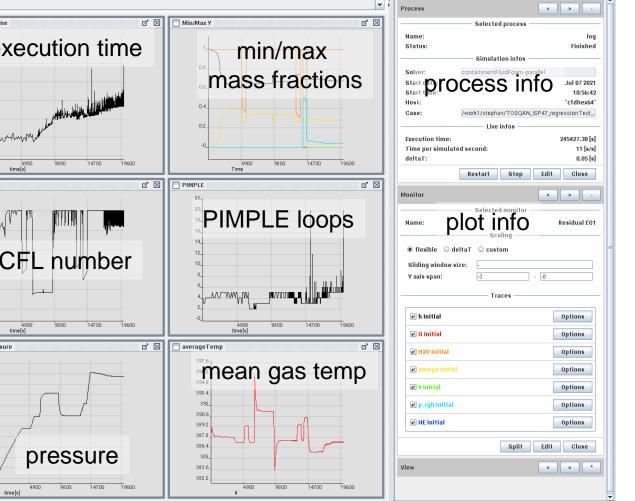
216000

189000

162000







#### IEK-14 Safety Research | S. Kelm et al. IAEA ONCORE TM, Politecnico di Milano, Italy, June 20-24<sup>th</sup> 2022

Slide 24

# **CONTAINMENTFOAM FRAMEWORK**

### **Solution Monitor**

- Based on OpenJDK and jchart2D (http://jchart2d.sourceforge.net/)
  - Steams OpenFOAM logs and functionObject output
  - Tab and Grid view
  - Flexible Regular Expression syntax
  - Filters, e.g. floating average, exponential smoothing, FFT..
  - Edit setup at runtime (selected dictionaries only)

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### OUTLINE

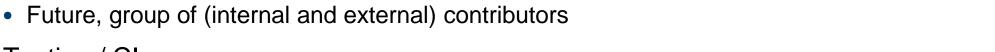
- Introduction
  - Background and Motivation
  - Strategy and General Considerations
  - Status of containment  $\nabla F$
- Open-source challenges
  - Maintenance, distribution
  - User-Developer interaction
- Best practices
- Summary and Perspective





#### **Our experiences**

- Documentation:
  - Do it in parallel to code development, e.g. using gitlab flavored markdown.
- Requirements:
  - Export control & dual use: needs time and careful argumentation with non-technical persons
  - Think of (internal and external) users!
  - Think of maintainability: aim for code-quality, harmonized code style, best practices etc.



Testing / CI:

**Our experiences** 

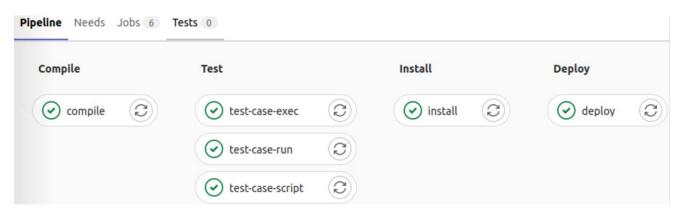
Management:

Currently, in personal union with group lead

Build test + simple test cases via CI pipeline; complex (costly) cases executed manually

**BEST PRACTICES IN NUCLEAR OS-PROJECTS** 

• Merge from 'feature' to 'development branch' only after independent review and testing (git 'approval')



### OUTLINE

- Introduction
  - Background and Motivation
  - Strategy and General Considerations
  - Status of containment  $\nabla F$
- Open-source challenges
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### **SUMMARY AND CONCLUSIONS**



- Development of containment  $\nabla F$  (mathematical Ambienter Ambien
- Coordinated effort to enable integration and balance of individual sub models and maintenance under the different time horizon of the individual contributors
- Productive version was released in 2021 <u>https://go.fzj.de/containmentFOAM</u>, currently small & known users group
- Measures taken to enable a productive user-experience and promoting a larger users group
  - Parallel development of Java based tools to assist users:
    - o cfGUI templated workflow to create new simulation setups
    - o cfSolutionMonitor graphical visualization of simulation logs for run-time verification and analysis
  - Communication via Mattermost chat, discussion forum
- Several best practices for software development employed, but limits exist due to manpower
- Applications: PWR flammable gas control (EU-AMHYCO), iPWR containment cooling (EU-SASPAM)

### ACKNOWLEDGEMENTS



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- Our contributors, partners and colleagues and beta testers
- The original developers, maintainers an contributors of OpenFOAM®





BACKUP

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# MAINTENANCE

### Design of containmentFOAM

- Not a stand-alone software, but add-on to OpenFOAM
- new functionality is added via
  - cloned and modified code (minor extensions)
  - separate base/derived classes (e.g., 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

