RETROSPECT, STATUS AND PERSPECTIVE OF THE DEVELOPMENT OF ‘CONTAINMENTFOAM’

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BACKGROUND AND MOTIVATION

The severe reactor accidents at Fukushima Daiichi Nuclear Power Plant (2011) have confirmed the need to understand the flow and transport processes of steam, combustible gases and radioactive fission products inside the containment and connected buildings. Experimental and analytical investigations on containment phenomena and their interaction with passive safety systems is a central part of the nuclear safety research conducted at JUELICH within the Helmholtz NUSAFE program ([1],[2]). This paper summarizes the design and implementation of *containmentFOAM* ([1],[4]), a tailored CFD solver and model library based on OpenFOAM® v6, which forms the basis for this R&D work.

The development of *containmentFOAM* is tightly linked with in-house and (inter)national experimental programs to ensure continuous validation along with the experimental progress. In turn, *containmentFOAM* supports the experimental test design and evaluation by providing detailed insights on the interaction of different transport phenomena. Finally, experimental results are transferred via validated models into containment application and can provide highly resolved insights to support the assessment of effectiveness of safety measures and possible combustion loads that may challenge the containment integrity.

The analysis of containment atmosphere mixing involves a multitude of different flow and thermophysical phenomena as well as technical systems to be modelled and linked together. This comprehensive development task demands a collaborative approach, which benefits from, and probably is only possible within an open-source model. In contrast to legacy codes, which are often protected by licences or export control regulations, open source enables international collaborations (e.g., with the Indian Institute of Technology Madras or within the OECD/NEA-NEST framework). It involves and motivates young researchers to contribute as their work and experience gained on the widely used OpenFOAM package can be further used without restriction and provides visible output. Furthermore, the implementation of an open-source model supports the dissemination and broader use of publicly funded research results. Besides being a ‘research product’, *containmentFOAM* aims to be an attractive platform for education, training, and maintenance of competence.

The paper will outline the general development considerations and strategy and briefly discuss the structure and status of containmentFOAM. Besides the framework, built to enable productive and consistent application is described. Concluding, the integration in the institutes work with respect to E&T including different levels of education (trainees to PhD candidates) is presented and the approach for dissemination is elaborated.

STRATEGY AND GENERAL CONSIDERATIONS

The development of *containmentFOAM* began in 2015 as an exploratory study in the frame of a Master Thesis and became a coordinated development project. Currently it has 14 active and former contributors, which in total added ~18.5 person years R&D. The development is mostly conducted by PhD students but also MSc students, interns, trainees, which demands efforts on integration and maintaining continuity. Coordination needs arise from the multi-scale and multi-physics nature of containment flows. I.e., all physical phenomena and their interaction must be considered to enable a representative simulation of an accident sequence. For the model development, this implies that models, developed by individual contributors, must be robustly coupled. Furthermore, the model basis must be well balanced in terms of accuracy and computational efficiency. In contrast to a multi-purpose CFD tool, the R&D focusses on substantiating and carefully extending a baseline model by documenting limitations rather than identifying an optimal model for a specific condition. This constraint also enables limiting the maintenance effort and user support.

To build on existing modeling experience, the first step was a thorough assessment of OpenFOAMs basic capabilities, available models and a transfer of the baseline model set developed in ANSYS CFX (v17.2) [5]. Together with a fundamental verification and validation this code forms the basis for the ongoing application-oriented validation and extension of the baseline model set. Besides the collaborative development and integration of physical models several cross-cutting tasks arise from the simulation workflow which demand a coordinated approach:

(a) Pre-processing: The case setup must reflect the latest developments and employ a consistent definition of the various sub models. Furthermore, the standards and common best practices need to be considered.
(b) Monitoring of the solution progress is of key importance to efficient use of the computational resources for long-running transient analysis.
(c) Similar post-processing steps (e.g., ‘evaluation of a mass balance’) need to be standardized using predefined ‘functionObject’ definitions and scripts.
(d) Parametric simulation runs (validation, DoE or uncertainty quantification) need automized workflows.

These common tasks led to the parallel development of a framework, which will be discussed later.

STATUS OF CONTAINMENTFOAM

Containment analysis primarily addresses the containment pressurization, the combustible gas mixing, and possible combustion loads during a severe accident. In recent years, CFD is increasingly employed to complement legacy codes with a higher level of spatial resolution and modeling details, with an explicit representation of relevant geometric aspects affecting the flow and transport phenomena. The development challenges of *containmentFOAM* are to:

(a) extend the application range of existing models to the prevailing flow conditions in containment studies (e.g., mixed convection),
(b) to achieve a balanced model set in terms of accuracy and efficiency. I.e., the accuracy of the full model set is limited by the coarsest modeling assumption, while the numerical effort is given by the most detailed model
(c) to consider all relevant physics and technical systems to enable a representative simulation

In *containmentFOAM* (detailed model descriptions are given in [3] or [4]), the containment atmosphere is described as a single phase (reacting) multi-component flow. A dedicated multi-species transport library was built on top of the OpenFOAM thermo and turbulence libraries for calculation of diffusive mass fluxes and corresponding enthalpy transport. Different models are provided to compute the effective binary diffusivities as well as the mixture transport properties. Furthermore, this library serves as a basis to integrate multi-phase phenomena such as wall condensation (e.g., [6]), fog formation and transport or aerosol transport. These phenomena are reduced to a single transport equation by utilizing a mixture model along with a drift flux approach and they interact with the gas phase via volumetric source terms, e.g., for the transfer of latent enthalpy or decay heat. It should be remarked that direct access to the solution algorithm enables a flexible and stable implementation of these source terms. Turbulent transport within the predominantly mixed and free convection flow is modelled by extending the available kω SST turbulence model with specific source terms to account for production and dissipation of turbulent kinetic energy in density gradients based on the simple and generalized gradient diffusion hypothesis. The initially cold containment structures represent significant heat sinks and are represented within the multi-region framework. As the flow is wall-bounded and driven by wall heat transfer, a scalable and consistent wall treatment was implemented extending established wall functions. Gas radiation significantly affects heat transfer in humid atmospheres and is modelled using a Monte Carlo transport solver, based on the Emission-based Reciprocity method. It was developed utilizing the Lagrangian library for the photon transport. A dedicated Statistical Narrow Band correlated-k model for the absorption characteristics of the participating media was formulated based on HITRAN data [7].

Currently, an application-oriented validation of containmentFOAM is conducted based on the ISP-37 (VANAM M3) test, which features a steam and aerosol release into the multi-compartment Batelle Model Containment (BMC) [8]. First results shall be presented at the technical workshop.

Being a multi-physics CFD package, OpenFOAM lacks models to represent technical systems and components, but provides interfaces to include them. The operational behaviour of passive auto-catalytic recombiners (PAR) for combustible gas management is integrated by coupling *containmentFOAM* with the mechanistic 2D PAR model *REKODIREKT*, using a domain decomposition approach and the file-based coupling scheme. Pressure dependent flow path (doors or burst foils) are modelled utilizing the activeBaffle functionality in OpenFOAM. Containment coolers were modelled using a porous media CHT approach.

Even though analysis of combustion processes and resulting loads is currently not further evaluated in containmentFOAM, the available combustion models in OpenFOAM can be utilized within its pressure-based solver. An alternative is to use the computed fields as an initial condition for a specialized solver like *ddtFOAM* [9].

CONTAINMENTFOAM FRAMEWORK

containmentFOAM is an expert tool, that includes several non-standard models and demands a skilled user. Furthermore, containment application requires the combination of multiple models to represent the underlying physics and safety systems. The single models are typically developed within individual PhD research projects and comprise comprehensive expert know-how (e.g., in the definition of numerical parameters or the combination of available sub-models). Their definition is done primarily within multiple text files, so-called dictionaries (see *FIG. 1* left), which may also involve links to other dictionaries. It is obvious that there is a certain potential for user dependent errors, resulting from a false or incomplete model definition or inconsistencies among the dictionaries. Classically, this can be done e.g., by comprehensive documentation (document or Wiki), commented dictionaries and tutorial cases. Nevertheless, such documentation cannot consider all details and dependencies and is often lagging the code development. For these reasons, the *containmentFOAM* package relies on a guided case setup process (see *FIG. 1* right).

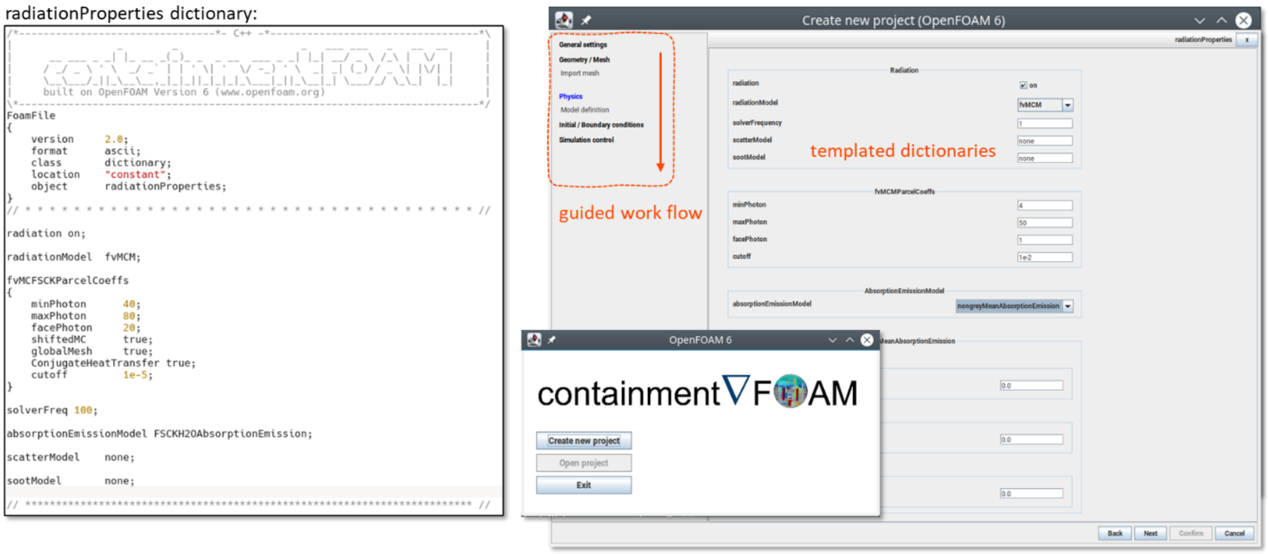

FIG. 1. Model definition in a dictionary (left), guided case setup (right).

It consists of an openJDK (GPL v2 [10]) based GUI, which guides the user through the case setup process. It is based on comprehensive JSON based templates, and rules that allow on the one hand a flexible extension and on the other hand to define logical dependencies to ensure consistent model definition in the various dictionaries. Furthermore, tooltips allow direct access to explanations. The definition of the JSON files includes the ‘best practices’ of the original model developer and are integrated along with the model development and V&V. The numerical methods and default settings specified for validation runs in [4] are the basis for the ‘simulation control’ template. By this means, the comparability of results obtained by different users and correct application of the models shall be maintained. Furthermore, this standardization is the only mean to ensure a certain quality of the simulation results and enable identification of model deficiencies.

A careful and continuous monitoring of a solution progress is of high relevance to identify possible issues in a long transient simulation early and thus use computational resources efficiently. For this purpose, a flexible solution monitor is developed on bases of the

JChart2D API (version 3.2.2 under LGPL, [11]) for live analysis of simulation progress in terms of convergence, performance and monitor variable histories (See *FIG. 2*).

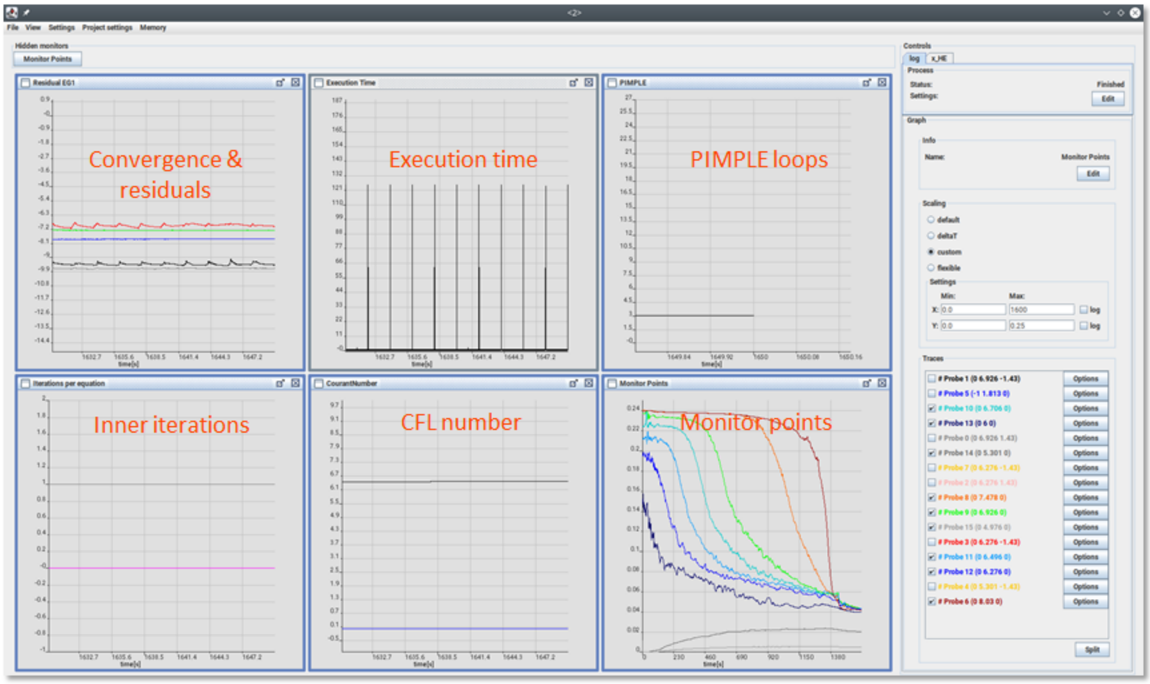

FIG. 2. Flexible solution monitor.

It uses a regular expression syntax to stream and evaluate all kinds of text-based output files produced by OpenFOAM, such as the solver log or functionObject output. Different filters, such as floating average or FFT can be flexibly combined to analyze the comprehensive solver output during run time and identify potential issues at an early stage.

During CFD model development and validation, there is the frequent need to prepare, run and evaluate parametric simulations, e.g., in case of inverse modeling, design space exploration or uncertainty quantification, which is realized by a slim python-based software.

The development of the framework is conducted primarily as part of student work, but also within the dual curriculum of the mathematical technical software developer trainees. Thus, it became an early starting point for undergraduate students to setting up CFD simulation workflow and scientific programming.

DISSEMINATION

As initially stated, the use of an open-source model is considered as a carrier to bring individual research into an application by a broader community. In this spirit, *containmentFOAM* is further developed to become an open basis to predict containment flows, pressurization, combustible gas and aerosol behavior and associated safety measures. Consequently, *containmentFOAM* is developed under the GNU Public License (GPL) v3. As it is developed within the context of nuclear safety engineering, export control compliance was addressed early, and a zero-notification was issued.

Currently, a beta version consisting of a baseline set of models is available for testing and feedback is requested to prepare a publicly available version. New model improvements and extensions are continuously. In the mid-term containmentFOAM shall become a part of the multiphysics simulation platform for education and research in nuclear applications, developed within the ONCORE initiative [12]. On the other side, it shall establish an open link to related non-nuclear research fields e.g., safety assessment of industrial processes or the applications of hydrogen as an energy carrier.

SUMMARY AND PERSPECTIVE

The paper summarized the development of the CFD package containmentFOAM for analysis of containment atmosphere transport processes. While many approaches are based on commercial multi-purpose CFD tools and limited to interfaces and built-in generic modeling capabilities. In contrast, *containmentFOAM* aims at providing a tailored and coupled model library for the specific conditions of accidental flows. The development is integrated in the institutes research work, but also in E&T with partner universities. While a first step aimed at building a representative and complete model set, focus of R&D now shifts towards code maintenance, validation, and application. This opens also doors for collaborations on the further validation, extension or application of the package.

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