Mobility Report for SEAKNOT-EU Project

Validation of MELCOR V2.2 for QUENCH-19 with FeCrAl Advanced Technology Claddings

Francesco Rosi

Mobility Details

- Sending Institution: Università di Pisa - Prof. Sandro Paci, Dr. Michela Angelucci
- Receiving Institution: KIT - Dr.-Ing. Fabrizio Gabrielli, Dr. Mauricio E. Cazado
- Mobility Period: 30/06/2025 – 19/12/2025

Introduction

Advanced Technology Fuel (ATF) cladding materials have gained significant attention in recent years due to their potential to enhance the safety margins of nuclear reactors, leading to intensive research and development. These materials aim to mitigate the in-vessel progression of severe accidents, by limiting the hydrogen generation and simultaneously preserving the cladding integrity at higher temperature and for a longer time.

Among the proposed ATF cladding candidates, FeCrAl alloys have shown to be a promising option, owing this to their high oxidation resistance in a wide range of temperatures, consequently offering a reduced hydrogen generation compared to conventional Zr-based claddings. Evaluating the capability of integral codes for severe accident analyses to reproduce ATF materials behaviors is a major concern in light-water reactor research at present.

This SEAKNOT mobility action had the objective of comparing the performance of MELCOR V2.2, a fully integrated severe accident code developed by Sandia National Laboratories, against the experimental results of QUENCH-19, a bundle test conducted in 2018 at the QUENCH large scale facility of Karlsruhe Institute of Technology (KIT). The mobility took place at the Institute for Neutron Physics and Reactor Technology of KIT, Germany, and was carried out in the framework of my master's thesis at University of Pisa, which is a requirement to be fulfilled for the completion of the degree.

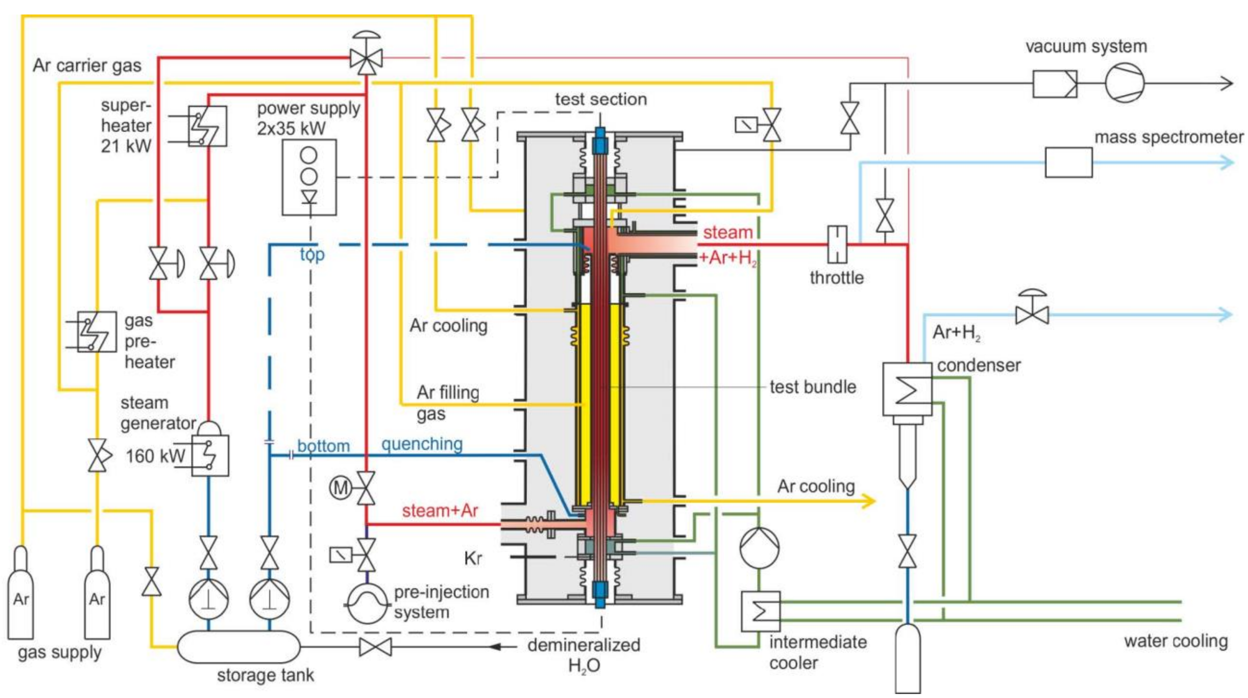

Figure 1 - QUENCH facility [1]

The experimental facility, shown schematically in Fig.1, is used to reproduce a Severe Accident (SA) in which a rod bundle is electrically heated, representing an uncovered core in a steam environment, followed by a quenching phase. Under these conditions, cladding temperature and hydrogen generation are measured and evaluated.

QUENCH-19 was the world's first bundle test simulating severe accident conditions with ATF cladding materials, and it was conducted using B136Y3, a FeCrAl alloy developed by Oak Ridge National Laboratory, USA. The bundle contains 24 approximately 2.5 m long FRS (Fuel Rod Simulators) (Fig.2) with FeCrAl cladding, that are electrically heated along a 1024 mm long region, and 7 unheated corner rods, entirely made of FeCrAl.

As shown in Fig.3, the rods are surrounded by an 89 mm outer diameter FeCrAl shroud with a 34 mm thick ZrO_2 insulation fiber, and a double walled cooling jacket.

Many thermocouples are inserted in the bundle and on the outer components to monitor temperatures during the sequence. The mass of hydrogen released is measured by a mass spectrometer, located at the off-gas pipe of the facility.

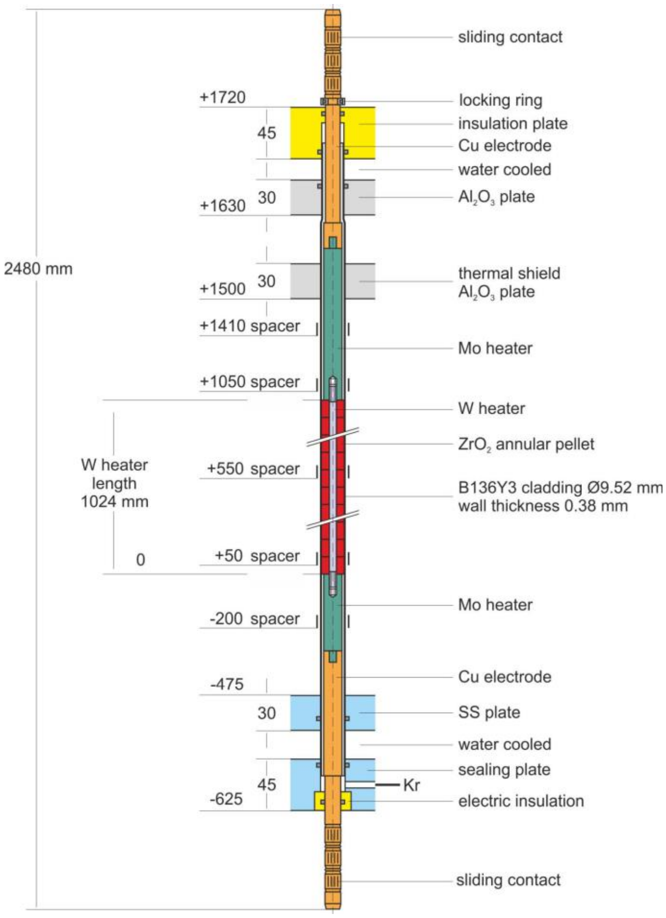

Figure 2 - QUENCH-19 FRS (Fuel Rod Simulator) [1]

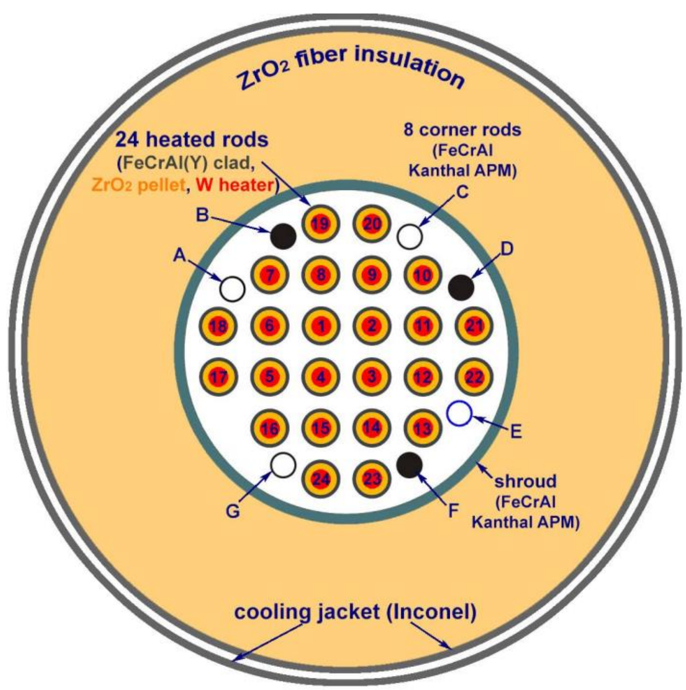

Figure 3 - Section of the QUENCH-19 test bundle [1]

The test sequence can be described by the power history in Fig.4 and the gas flow rates in Fig.5.
The transient can be split into 4 separate stages:

1. Pre-oxidation: 0 – 6018 s
2. Power transient: 6018 – 7127 s
3. Constant power: 7127 – 9115 s
4. Water quenching: 9115 – 9285 s

The power profile during the pre-oxidation phase of the QUENCH-19 experiment was designed to match the one of the Zr-alloy reference test QUENCH-15.
All the data on electrical power, flow rates and TCs temperatures was provided by KIT.

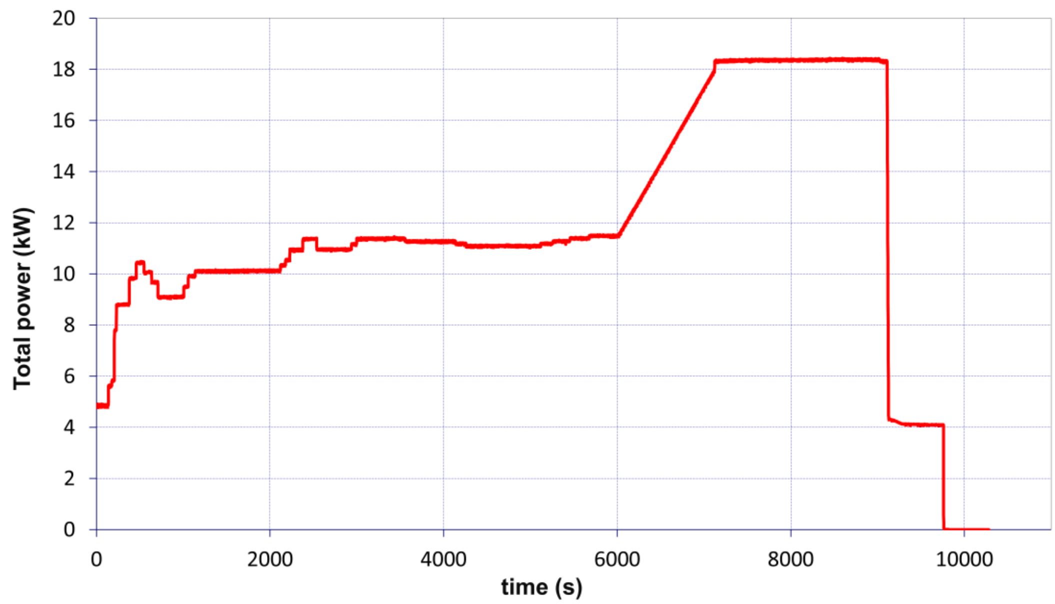

Figure 4 - Electrical power history

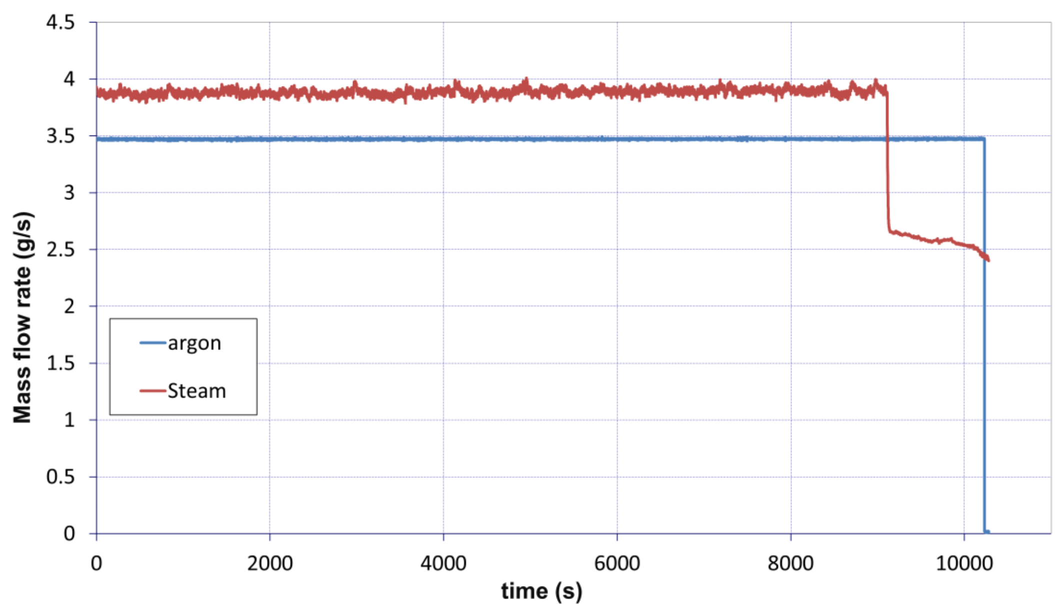

Figure 5 - Gas flow rates

Summary of the work performed

First, a literature review was conducted on FeCrAl (and its oxides) **thermophysical properties** and **oxidation behavior**. Gathering this information was crucial for developing a model of these new materials to be implemented in MELCOR. In fact, the code has default properties for the metallic phase and for a FeCrAl oxide that consists of a single oxide phase representing all possible oxides formation. Nevertheless, because the main goal of this work was to validate the code performance of the specific characteristics of QUENCH-19, it was decided to tailor the properties to the specific alloy B136Y3 when they were available in the open literature [2-6]. The oxide properties used were the ones by default. Regarding the oxidation behavior, all the data was taken from the results of KIT separate effect test on B136Y3 [7].

Then, a **nodalization** was created for the QUENCH-19 test bundle, according to the data and dimensions from the official KIT experimental report. Different versions of this model were prepared and tested to reach a configuration that was at the same time realistic, efficient and compatible with MELCOR code constraints.

This nodalization was then used as a starting point and template to produce a complete MELCOR **input deck**. MELCOR latest version, **MELCOR v.2.2 R2025** [8,9], was used for this work, due to its newly introduced functions regarding the oxidation behavior of user-defined materials.

An extensive process of trial and error was required to achieve a stable and satisfactory **Best Estimate** result. This involved the creation of many input decks, exploring the capabilities and the limitations of MELCOR in modeling both an electrically heated experimental facility (instead of a full-scale reactor) and FeCrAl ATF (instead of the well characterized Zr alloys).

Among the many challenges encountered during this part of the work, four were the most significant:

1. **Radial nodalization of the "core":** while MELCOR allows the user to radially discretize the core in multiple rings, only 2 of those rings can contain electrically heated material. This is a limitation regarding the capability of the code to produce results that closely match the experimental value of temperature, which can present a significant gradient across the core radius. Furthermore, oxidation (and thus, hydrogen production) is a temperature dependent phenomenon, and it was found that, in the hottest levels, even a slight temperature increase would significantly accelerate this process. To address this issue, multiple radial configurations were tested until satisfactory results were reached.
2. **SH (shroud) component and bypass:** MELCOR COR package contains, among all the ones available, a component dedicated to the shroud (SH), that can allow the user to represent the "shroud" present in the QUENCH-19 experiment. However, this COR component requires the definition of a bypass control volume around it, which does not represent any physical part of the experiment. Furthermore, while MELCOR provides a tool to model heat conduction from certain COR components to external heat structures, the SH component cannot be selected as an input for this feature. While other possibilities were explored, it was decided to include a virtual bypass volume in the model, since it provided results that were stable and coherent with the experimental data. This feature consisted of seven Argon-filled control volumes with a thickness of 0.5 mm

stacked on top of each other, representing a gas-filled annulus between the shroud and the ZrO_2 fiber insulation layer.

3. **GOX (generalized oxidation model) implementation:** This MELCOR model allows the user to introduce new oxidation reactions or modify existing ones. Many parameters can be specified, such as the stoichiometry, the heat of the reaction and the parabolic rate constant (Eq.1). This temperature dependent kinetics constant (K) directly correlates to the mass of oxide and H_2 produced by the reaction. This kinetics rate constant is described with the Arrhenius constants *A* and *B*, which also depend on the temperature range and can be independently specified in the input deck. In addition, the parabolic rate constant must be considered for mass of **metal** reacted, instead of oxygen mass gain. The model allows the user to split each reaction into many temperature ranges, but also to model the oxidation of a material with multiple reactions, which would be more realistic for FeCrAl: during its oxidation in steam, in fact, all three of its main constituents (Iron, Chromium and Aluminum) can oxidize, depending on the temperature. Unfortunately, using this last feature made the simulations long and unstable and produced inconsistent results. It was therefore decided to use a single reaction with the stoichiometry of Magnetite (Eq.2) and to assign different values for *A* and *B* in separate temperature ranges, based on the reaction kinetics that were observed at that temperature during separate effect tests. The resulting parabolic rate constant is compared to experimental data in Fig.6.

$$\frac{d(W^n)}{dt} = K(T) \quad ; \quad K(T) = Ae^{\left(-\frac{B}{T}\right)}$$

Eq. 1 – Parabolic rate equation and parabolic rate constant for the oxidation

$$3\mathrm{Fe} + 4\mathrm{H_2O} \rightarrow \mathrm{Fe_3O_4} + 4\mathrm{H_2}$$

Eq. 2 – Magnetite oxidation reaction

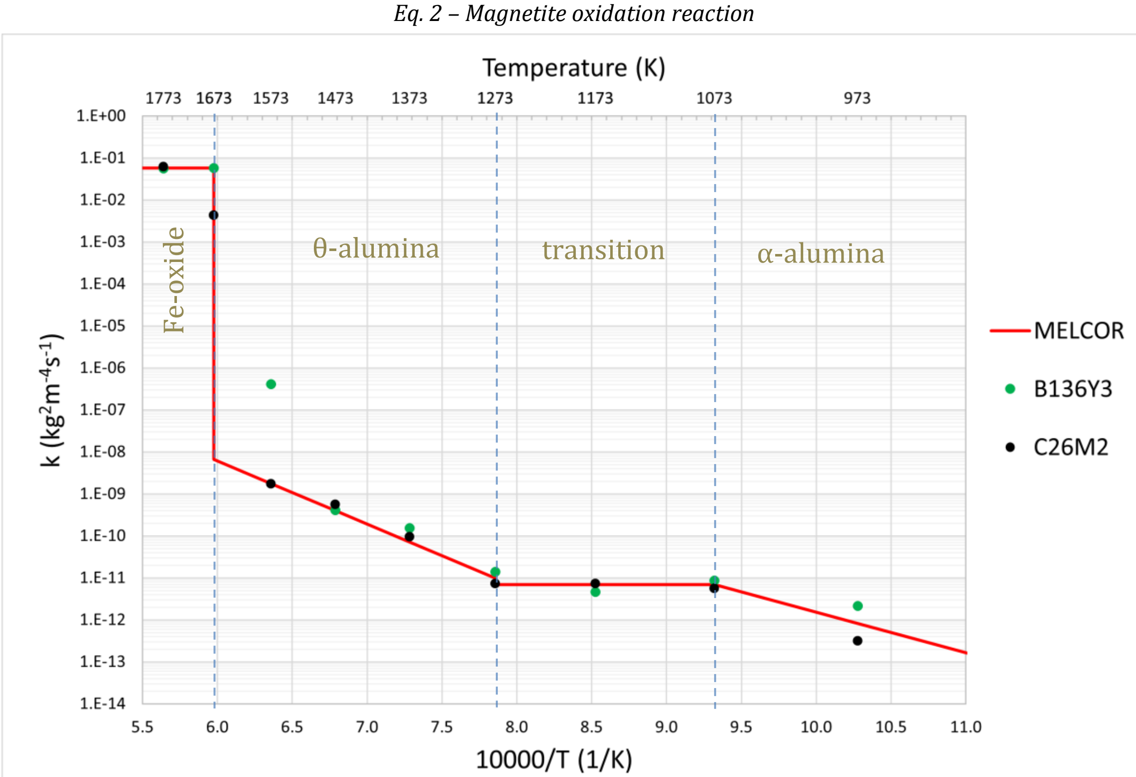

Figure 6 - Parabolic rate constants of FeCrAl alloys

4. **Stainless steel TC sheaths:** The QUENCH-19 report estimates that around 2 of the total 9.2 grams of H_2 produced should be attributed to the oxidation of thermocouples. The TCs inside the bundle are, in fact, enclosed in stainless steel sheaths, some of which showed significant degradation, melting and oxidation in the post-test examination. Since the thermocouples were not physically modelled in the input deck, the hydrogen produced by the oxidation of their sheaths has been calculated using available data: the temperatures in each cell were collected from the simulation results, the number of thermocouples and their exposed surface were derived from the KIT report, and a standard correlation for the oxidation of SS was used. This hydrogen mass was then added to the total H_2 production of the simulation, which only considered the oxidation of FeCrAl.

The results of the hydrogen production simulations show that those performed with MELCOR without accounting for the thermocouple sheath (SS) predict approximately 6.5 g of hydrogen at the end of the transient. However, when the additional hydrogen generated by the thermocouples is included, calculated from the thermocouple temperature evolution provided by the code, the total increases to 9.1 g, which is in very good agreement with the experimental measurement of approximately 9.2 g. Furthermore, a comparison of the simulated and measured temperature evolution showed satisfactory overall agreement, despite the expected deviations associated with modelling simplifications and the previously discussed limitations. These results demonstrate that MELCOR can adequately reproduce the key conditions and results of the QUENCH-19 experiment. The outcomes presented here constitute the technical basis for foreseen scientific publications (conference and journal) currently being planned by KIT.

Finally, a **U&SA** (**uncertainty and sensitivity analysis**) was performed, to evaluate the impact of the uncertainties of the oxidation correlation on hydrogen production. Two parameters were chosen to be studied:

- **TSWITCH**: The temperature at which the biggest jump in the parabolic rate constant occurs, switching from θ-alumina to iron oxide kinetics, which can be clearly noticed in thew logarithmic plot in Fig.6. A range of ±50 K was selected for this parameter.
- **AGAIN**: A constant coefficient to be included in the parabolic rate constant calculation, as shown in Eq.3. A range of [0.85; 1.15] was chosen for this parameter.

$$K(T) = AGAIN \cdot Ae^{\left(-\frac{B}{T}\right)}$$

Eq. 3 – Modified parabolic rate constant with the uncertainty parameter AGAIN

To ensure an equal probability for each value within the specified ranges, a **random sampling** approach was adopted, where the input parameters were selected according to a uniform probability distribution using a python script. After producing 100 samples, in which the two parameters were varied simultaneously, an equal number of input decks were created and simulations were performed.

The only FoM (Figure of Merit) selected was H_2 production, since the two parameters considered almost exclusively affect that output variable.

The simulations results were analyzed and compared using **Spearman** correlation. The results show that, while both parameters have a significant effect at different simulation times, TSWITCH is the one with the most overall impact on hydrogen production.

Conclusions

A MELCOR input deck was developed through an iterative process during which multiple configurations were assessed and progressively improved. This approach was essential for understanding the sensitivities of both the code and the model and for selecting a consistent and robust configuration.

Despite some deviations, to be attributed to the limitations in the core nodalization, the Best Estimate results show good agreement with the experimental data provided by KIT regarding the most relevant parameters, such as hydrogen production and cladding temperatures. Therefore, MELCOR code is able to adequately reproduce the oxidation behaviour of FeCrAl ATF cladding in the QUENCH-19 conditions.

An uncertainty and sensitivity analysis was performed on two parameters affecting the oxidation correlation. The analysis shows that changing the parameter that controls the temperature of the switch from alumina to Fe-oxide oxidation kinetics has the strongest effect on H_2 generation.

This mobility action has been a unique opportunity for me to gain extremely valuable knowledge on severe accidents and system codes, as well as uncertainty quantification. I had the chance to work, together with experts and professionals in the field, on a topic that is both exciting and very much relevant for nuclear safety research at present.
Finally, during to this experience I was able to meet the members of the Reactor Physics and Dynamic Group at KIT, who have been welcoming and supportive of me and my work since my first day there.

I am thankful to SEAKNOT, to the Institute for Neutron Physics and Reactor Technology (INR) of KIT, and to University of Pisa (especially my professor Sandro Paci and my supervisor Michela Angelucci) for the opportunity to carry out this mobility action and for supporting me through it, and I am determined to keep working in this field in the future.

Bibliography

[1] J. Stuckert, M. Große and M. Steinbrück, “Results of the bundle test QUENCH-19 with FeCrAl claddings,” Karlsruhe Institute of Technology, Karlsruhe, 2022.

[2] P. Aragón, F. Feria and L. E. Herranz, "Modelling FeCrAl cladding thermo-mechanical performance. Part I: Steady-state conditions," Progress in Nuclear Energy, vol. 153, p. 104417, 2022.

[3] P. Aragón, F. Feria and L. E. Herranz, "Modelling FeCrAl cladding thermo-mechanical performance. Part II: Comparative analysis with Zircaloy under LOCA conditions," Progress in Nuclear Energy, vol. 163, p. 104838, 2023.

[4] K. G. Field, M. A. Snead, Y. Yamamoto and K. A. Terrani, "Handbook on the Material Properties of FeCrAl Alloys for Nuclear Power Production Applications (FY18 Version: Revision 1)," ORNL, United States, 2018.

[5] "NIST Chemistry WebBook, SRD 69," National Institute of Standards and Technology, [online]. Available: https://webbook.nist.gov/

[6] “IAEA Thermo-Physical Materials Properties Database” International Atomic Energy Agency. https://nucleus.iaea.org/sites/therpro

[7] C. Kim, C. Tang, M. Große, Y. Maeng, C. Jang and M. Steinbrück, "Oxidation mechanism and kinetics of nuclear-grade FeCrAl alloys in the temperature range of 500-1500 °C in steam," *Journal of Nuclear Materials,* vol. 564, p. 153696, 2022.

[8] L.L. Humphries, B.A. Beeny, K.N. Belcourt, F. Gelbard, T.C. Haskin, J. Phillips, “MELCOR Computer Code Manuals Vol. 1: Primer and Users' Guide Version 2.2 r2024.0”

[9] L.L. Humphries, B.A. Beeny, K.N. Belcourt, F. Gelbard, T. Haskin, J. Phillips, “MELCOR Computer Code Manuals Vol. 2: Reference Manual Version 2.2 r2024.0”