MELCOR Validation Against the QUENCH-19 Experiment and Outlook on ATF-Related Activities

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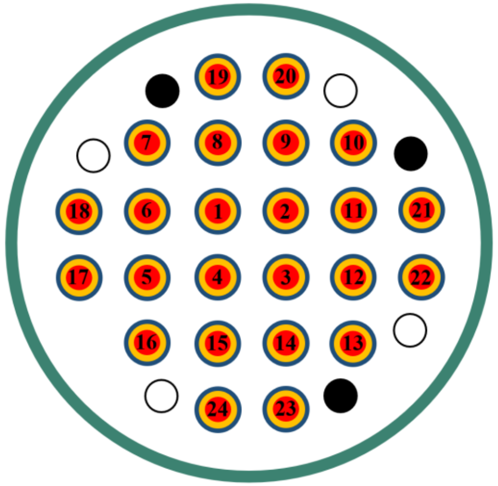
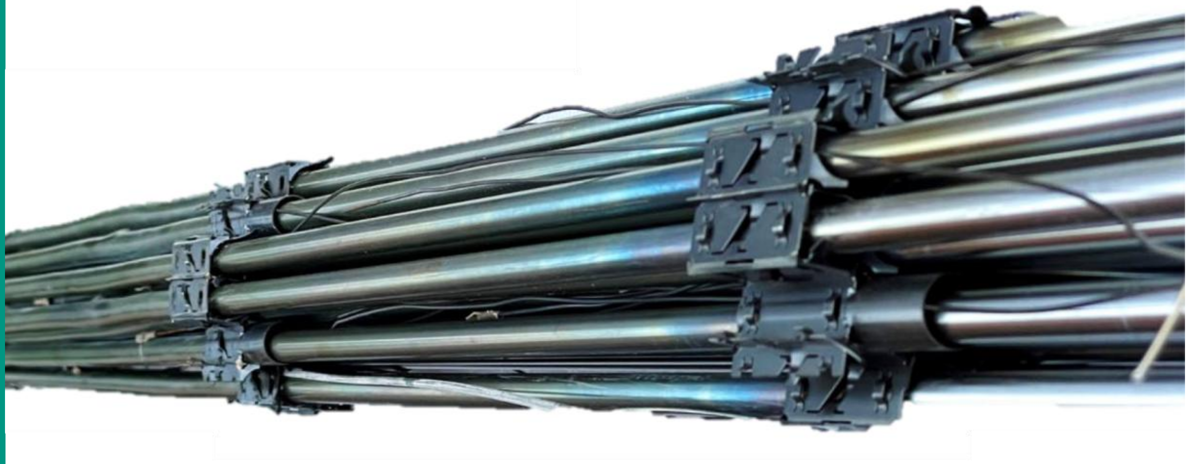




(Steinbrück, 2022)

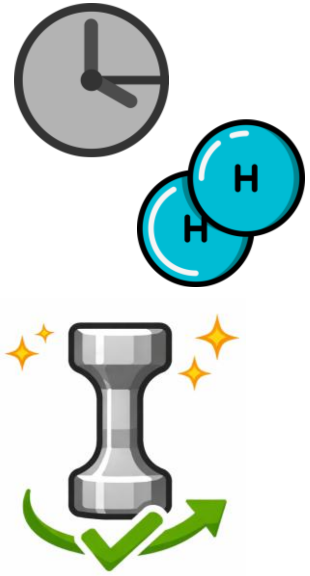
Content

Introduction

Advanced Technology Fuels

IAEA definition: *"Enhanced accident-tolerant fuels (ATFs) are fuels that can tolerate a severe accident in the reactor core for a* ***longer time period*** *than the current UO_2 zirconium alloy fuel system, while* ***maintaining or improving*** *the fuel performance during* ***normal operations and operational transients****."*

Current ATF designation: Advanced Technology Fuel



Desired characteristics

- Delay degradation and extend coping time.
- Reduced steam reaction kinetics and lower hydrogen generation rate.
- Maintaining or improving FP behaviour, thermomechanical properties

Several Experiments and Projects on ATF

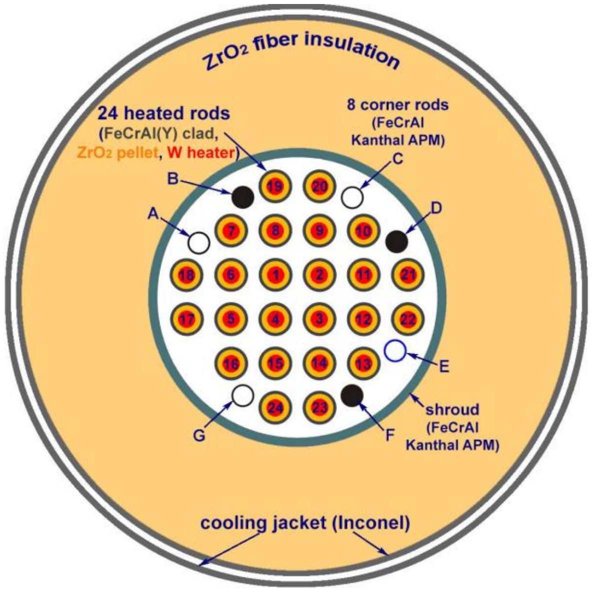
- **QUENCH-19: FeCrAl**
- OECD/NEA QUENCH-ATF: Cr-Coated Zr
- CROCODOX: Cr-coated Zr
- IAEA ACTOF, ATF-TS

QUENCH-19 Bundle Test

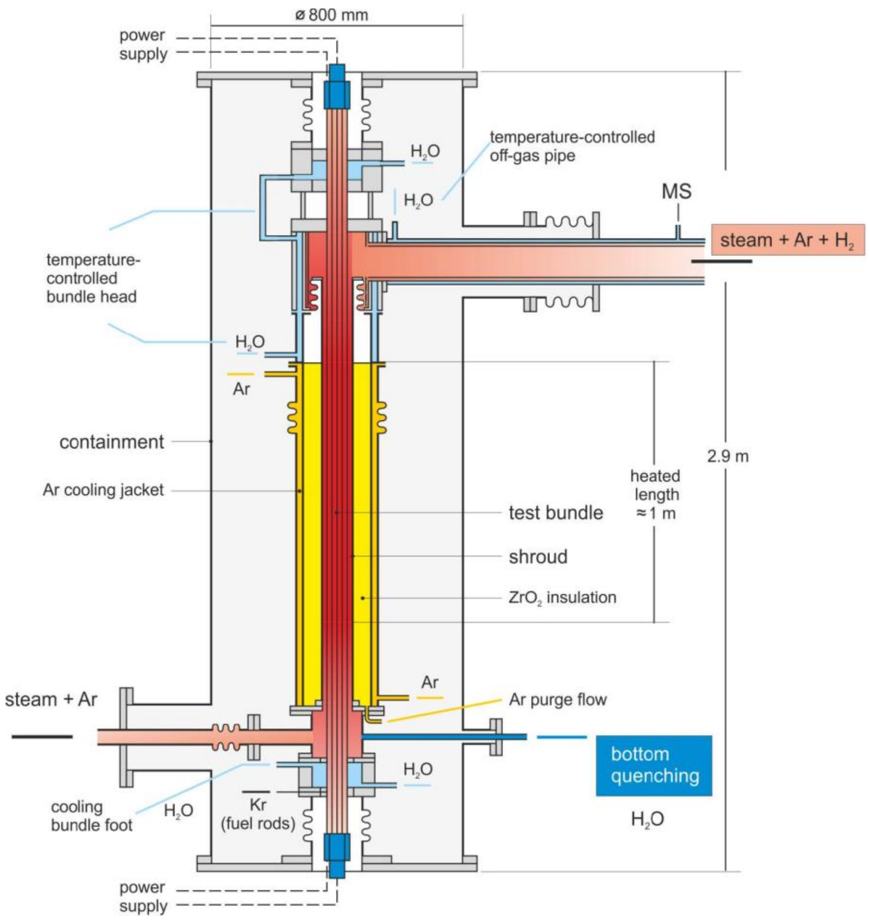
QUENCH Facility at KIT

QUENCH-19 Experiment

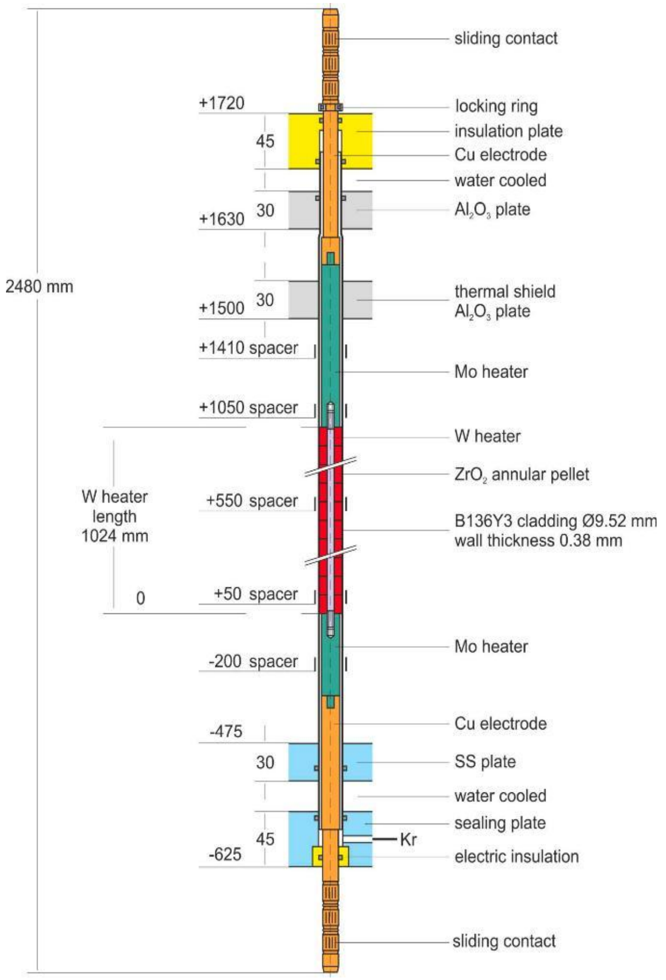
The first integral bundle test worldwide using ATF cladding, performed at the QUENCH facility (KIT, 2018) with FeCrAl alloy (B136Y3) rods.



Section of the QUENCH-19 test bundle (Stuckert, 2022)

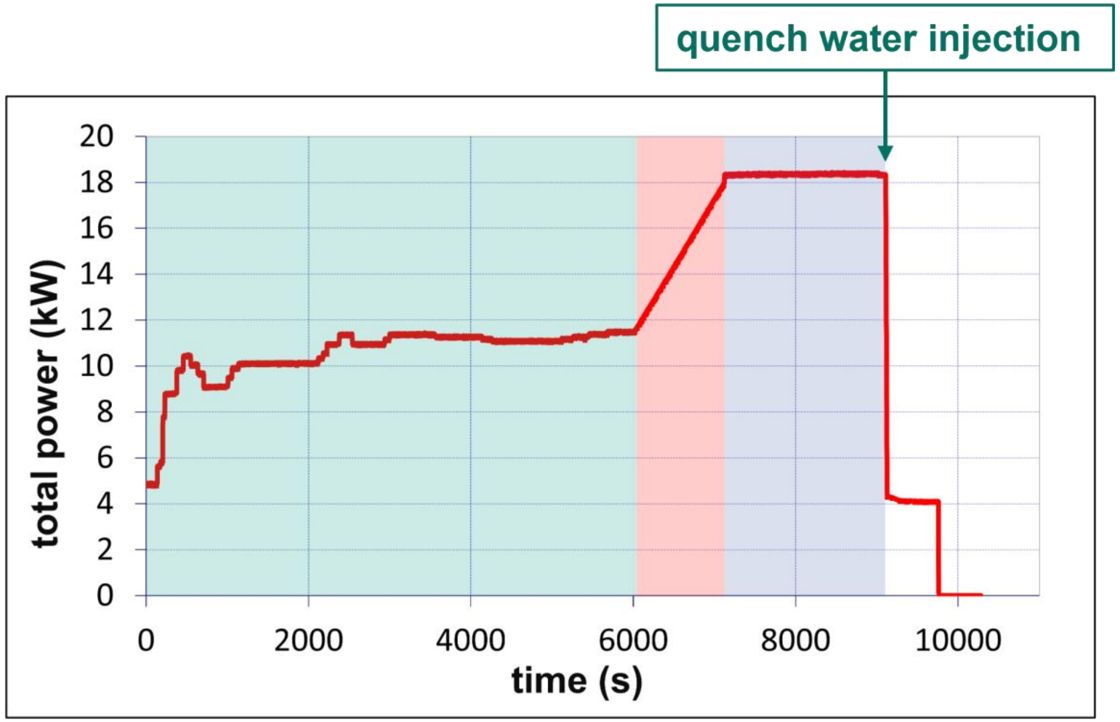


QUENCH-19 Test section (Stuckert, 2022)



Heated fuel rod simulator (Stuckert, 2022)

QUENCH-19 Bundle Test



QUENCH-19 Electric power (Rosi, 2026; Stuckert, 2022)

Experimental Stages – QUENCH-19

Stage	Duration	Notes
Pre-oxidation	0 – 6018 s	Similar to QUENCH-15
Heat-up	6018 – 7127 s	Similar to QUENCH-15
Extended heating	7127 – 9100 s	Constant electrical power
Quench	~9115 – 9285 s	Similar to QUENCH-15

- **Pre-oxidation**: a protective Al2O3 layer was formed under steam/argon flow.
- **Heat-up**: electrical power was ramped up to simulate rapid core heating up to 1470 of PCT.
- **Extended heating**: constant maximum power up to ~1810 K.
- **Reflood and quench**: water injection leading to bundle quenching.

(Rosi, 2026)

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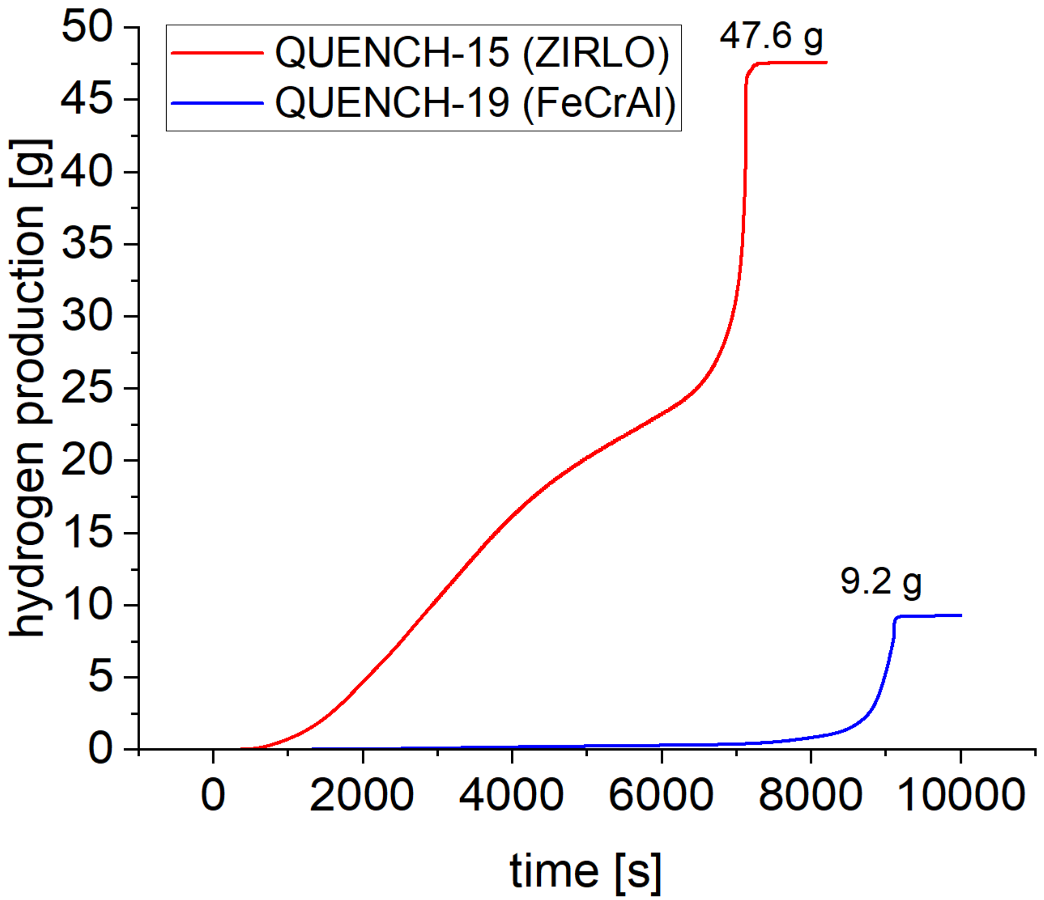
QUENCH-19 Bundle Test

Main findings

- No temperature runaway during transient when compared to ZIRLO reference, and max. temperatures ~200 K lower in the pre-oxidation phase.
- Large hydrogen reduction: **9.2 g vs 47.6 g (≈-80%).** Lower peak release rate during reflood.
- Oxidation escalation after Al_2O_3 failure (~1650 K).
- Circumferential breaks due to higher thermal expansion of FeCrAl and local melting.



Hydrogen generation comparison between ZIRLO and FeCrAl cladding (Stuckert, 2022)

FeCrAl Cladding Concept

- Fe-based alloy with 12 – 24 wt% Cr and 3 – 6 wt% Al.
- Nuclear grade FeCrAl: 10 – 13 wt% Cr and 5 – 6 wt% Al. Additional additives to improve oxidation resistance and mechanical properties: Mo and Y.

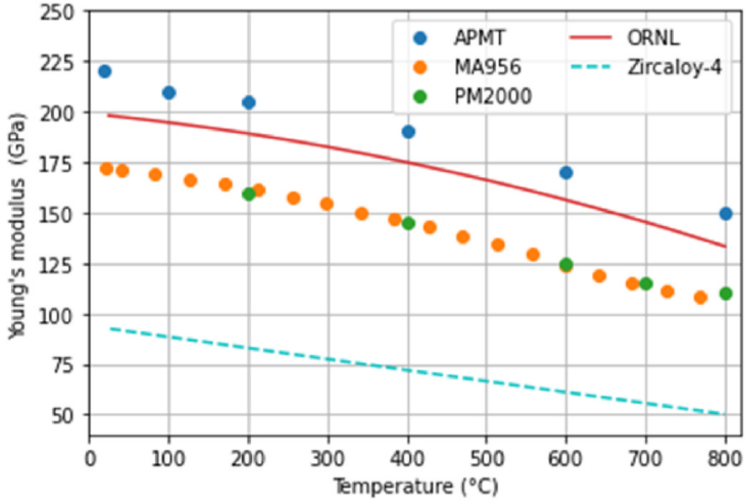
Alloy /wt%	Fe	Cr	Al	Mo	Y	C	Si
B136Y3	Bal.	12.97	6.19	-	0.03	<0.01	-
C26M2	Bal.	11.87	6.22	1.98	0.03	<0.01	0.2

Advantages

- Superior oxidation resistance at high temperatures due to the formation of a protective layer of Al_2O_3: strong protection below 1300 °C.
- Superior mechanical properties when compared to Zr alloy.
- Lower hydrogen generation under steam oxidation.

Disadvantages

- Higher neutron absorption cross-section than Zircaloy: cladding thickness must be reduced.
- Tritium permeability due to lack of hydrogen isotopes trapping, but lower than pure Fe.
- Under neutron irradiation, FeCrAl with high Cr content (20-22 wt%) is susceptible to Cr-rich α' phase → irradiation embrittlement.
- Interaction between UO_2 and FeO forming an Eutectic at ~1335°C



Young's modulus as a function of temperature (Aragon, 2022)

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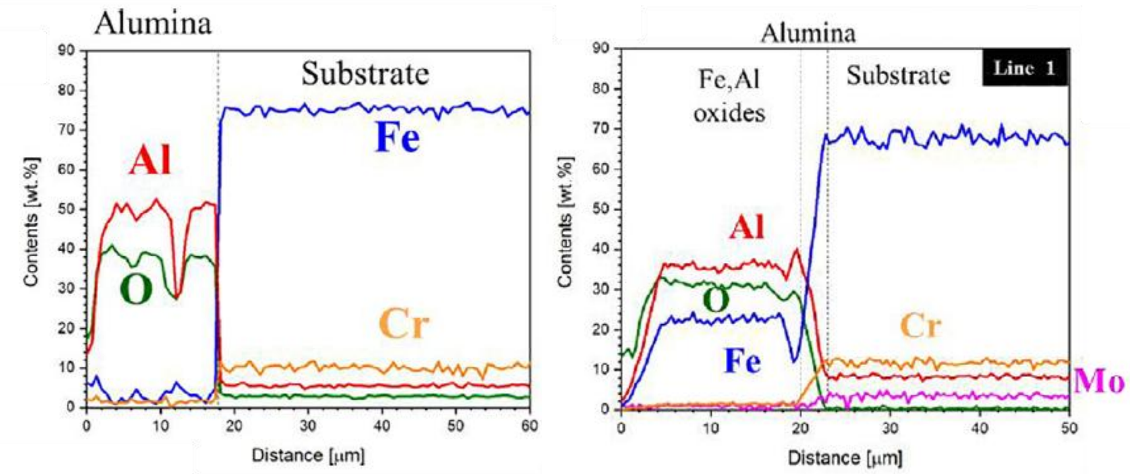
FeCrAl Cladding Concept

High-Temperature Steam oxidation

SETs at KIT QUENCH



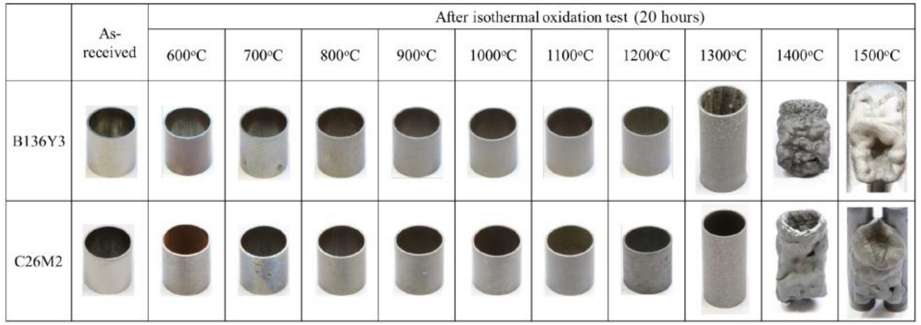
Elements profile along the sample thickness. Left: B136Y3 isothermal test at 1300°C. Right: C26M2 isothermal test at 1500°C.

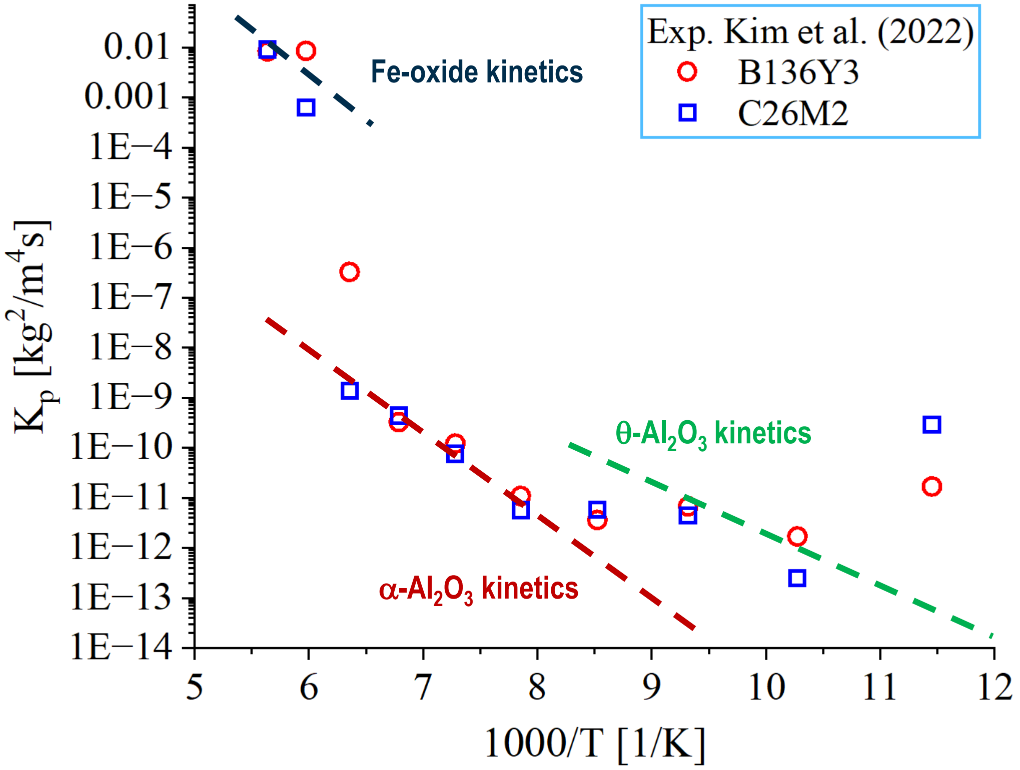
≤1300°C: Aluminum oxidation

>1400°C: Iron oxidation dominates the reaction

The general correlation for oxygen mass gain is:

$$k_p\left[\frac{kg^2}{m^4 s}\right] = \begin{cases} 5.3758\times10^{-3}\exp\left(-\frac{184730\ [J/mol]}{RT}\right), & 873\ K < T < 1173\ K \quad (\theta - alumina) \\ 4.69156\times10^{-12}, & 1173\ K \le T \le 1273\ K \quad (intermediate\ T) \\ 5.0176\exp\left(-\frac{287748\ [J/mol]}{RT}\right), & 1273\ K < T < 1648\ K \quad (\alpha - alumina) \\ 2.4\times10^{8}\exp\left(-\frac{352711.2\ [J/mol]}{RT}\right), & T \ge 1648\ K \quad (FeO\ melting\ point) \end{cases}$$





Parabolic rate constants of B136Y3 and C26M2 as a function of temperature with the parabolic constants of Fe-oxide , α-alumina and θ-alumina (Kim, 2022).

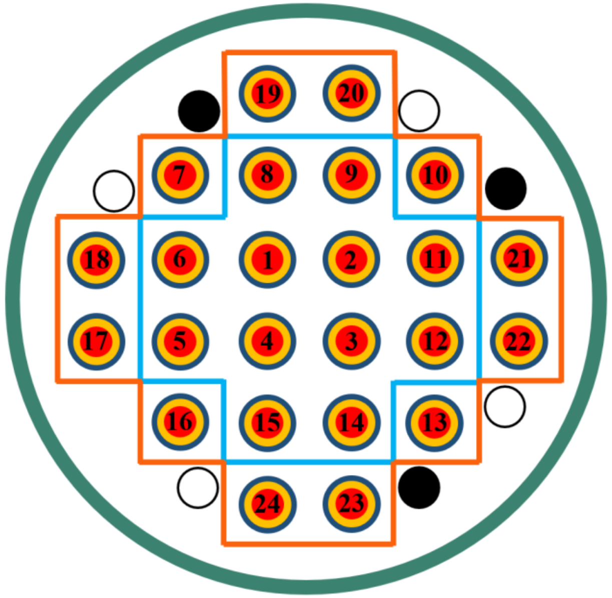
MELCOR Modelling

General Nodalization

- The nodalization was adapted from previous QUENCH models and extensively modified to reproduce the specific conditions of the QUENCH-19 experiment.
- Therefore, the model is not generic, but **strongly tailored to the geometry, boundary conditions, and operational sequence of the test**.

COR Radial Nodalization

- The bundle was discretized into multiple radial rings.
- At the time of the study, only **two rings were electrically heated**, limiting the reproduction of radial temperature gradients.
- Additional heated rings may be possible with alternative MELCOR input options.



Radial Nodalization

Radial Nodalization

- **Ring 1:** 12 Rods + Grids
- **Ring 2:** 12 Rods + Grids
- **Ring 3:** 7 Corner Rods + Shroud

(Cazado et al., 2026a; Rosi et al., 2026; Angelucci et al., 2026)

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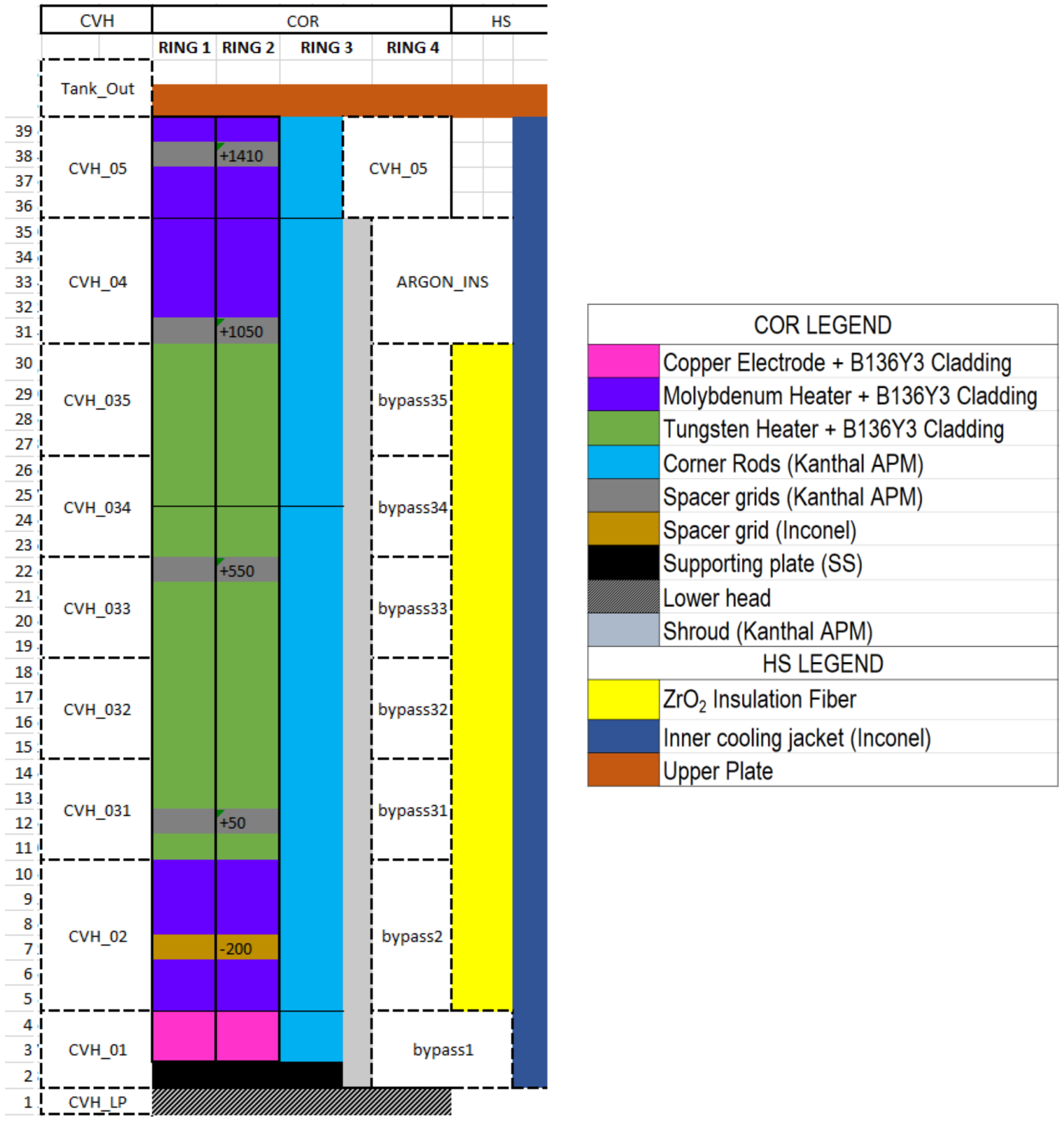
MELCOR Modelling

COR Axial Nodalization

- Discretization was defined based on MELCOR code requirements and the actual bundle geometry

Level 1: Lower Plenum
Level 2: Core Supporting Plate
Level 3-39: QUENCH19 bundle



(Angelucci et al., 2026)

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MELCOR Modelling

CVH Nodalization

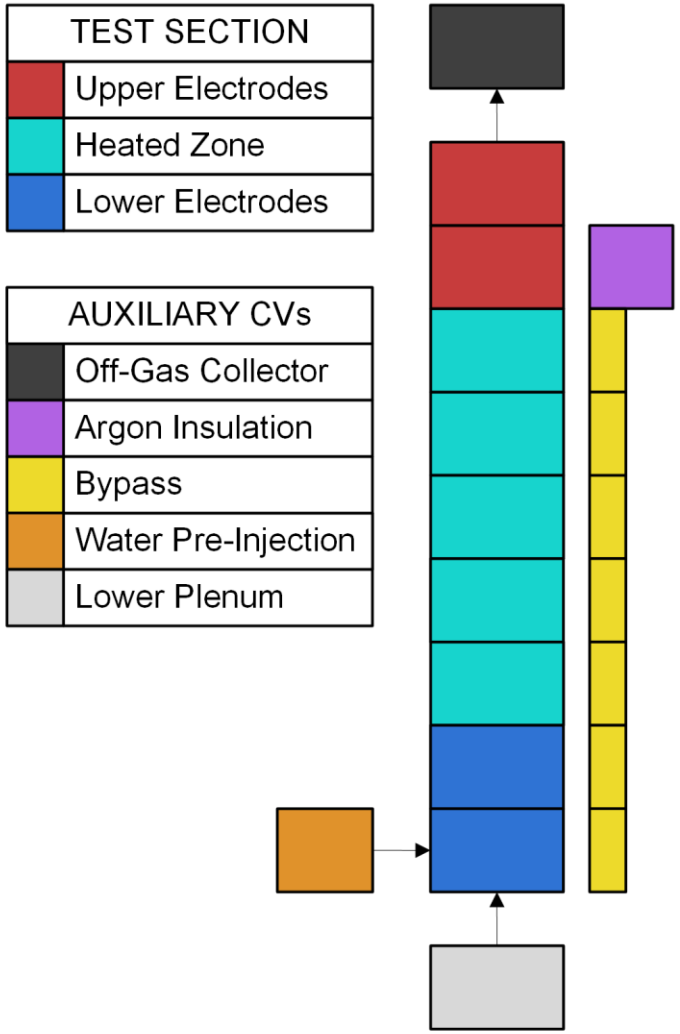
Test Section is divided axially:

- Upper electrodes zone
- Heated zone
- Lower electrodes zone

Additional volumes for LP, Containment, Off-Gas collector, Argon insulation.

Shroud-to-insulation heat conduction was simulated with a “Virtual“ 0.5mm thick Bypass volumes between them.

(Cazado et al., 2026a; Rosi et al., 2026)



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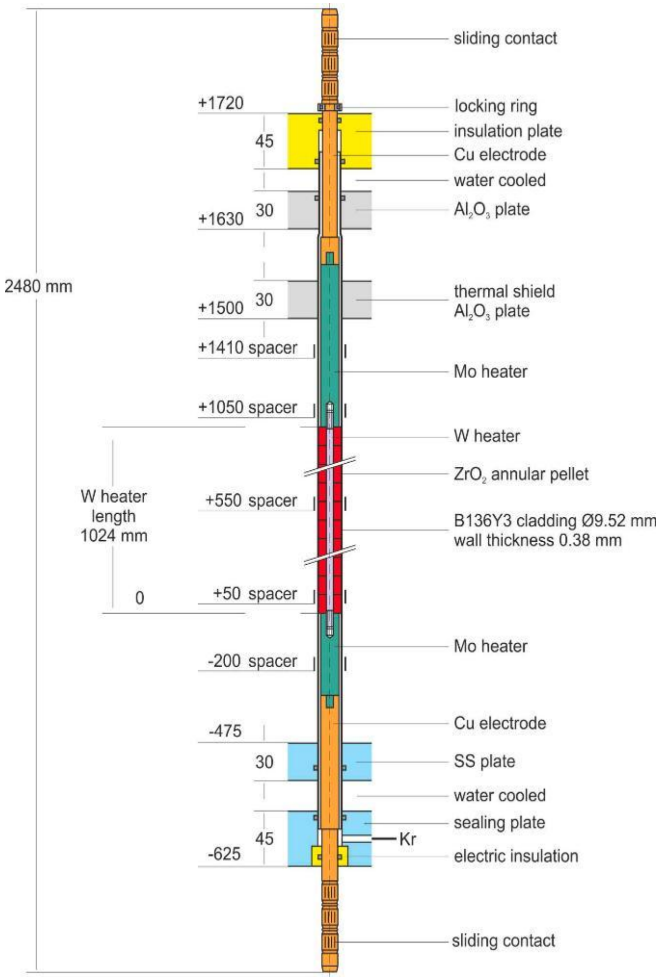
MELCOR Modelling: Materials

- **W**, **Mo**, and **Cu** (heater/electrode) properties defined through the MP package as function of temperature.
- **ZrO_2 annular pellets** around the heaters modelled via UO_2 as a placeholder material with ZrO_2 properties.
- **B136Y3** material defined as the oxidizable user material. Properties obtained from literature and KIT data (Aragon, 2022; Field, 2018) Claddings, corner rods, shroud, and spacer grids are represented with this user-defined material.
- **B136Y3OX** oxide material represented using MELCOR default properties



Heated fuel rod simulator (Stuckert, 2022)

(Cazado et al., 2026a; Rosi et al., 2026; Angelucci et al., 2026)

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MELCOR Modelling: Materials

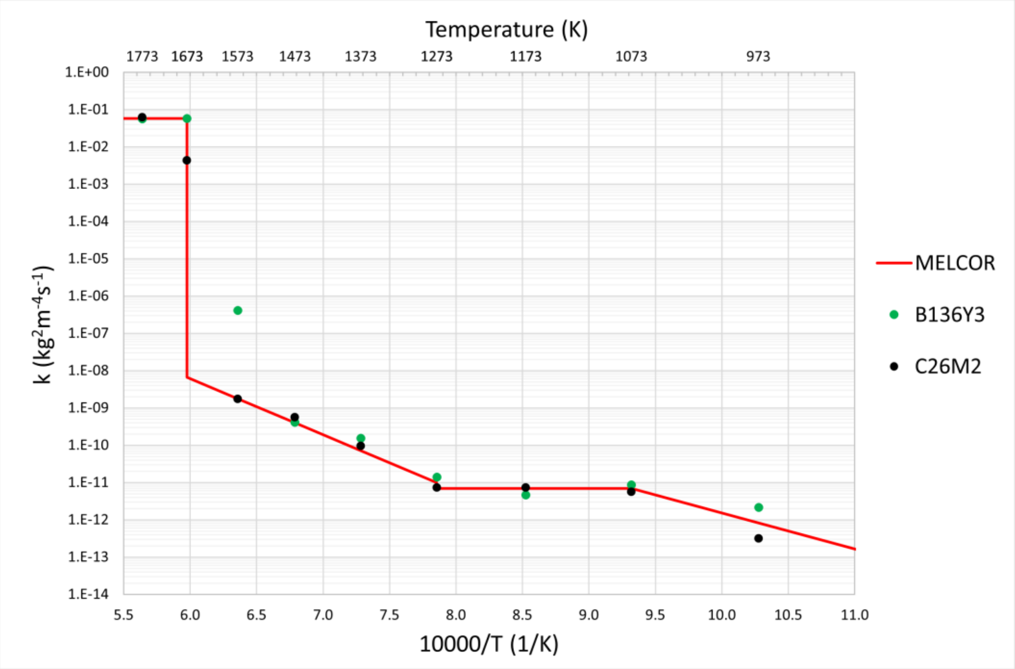
FeCrAl Oxidation

- A user-defined **GOX** (Generalized Oxidation Model) was used.
- The **GOX** model accepts separate reaction equations, but only one equation was used with kinetics depending on the temperature ranges.

Stoichiometry and heat of the reaction of magnetite (Fe_3O_4)

$$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$$

- The reaction rates for θ-alumina, α-alumina and magnetite were adapted based on the SET conducted at KIT: Arrhenius parameters for mass of metal reacted is required.
- The QUENCH-19 alloy, B136Y3, was used as the reference for the parabolic oxidation rate constant in the Fe-oxide regime.
- A sharp transition occurs at ~1673 K, from θ-alumina to Fe-oxide.



Parabolic rate constants of FeCrAl alloys

(Cazado et al., 2026a)

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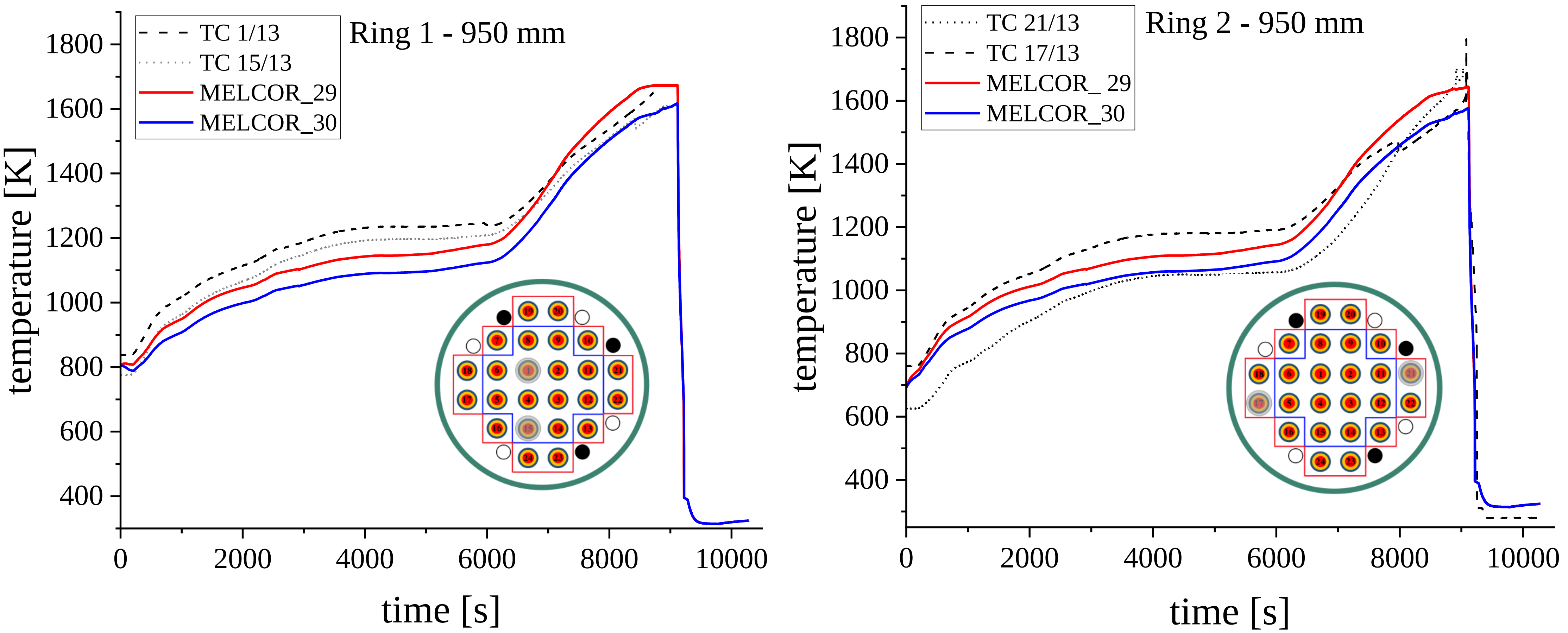
Simulation Results

Temperature Evolution – 950 mm elevation



(Cazado et al., 2026a)

Cladding temperature at 950 mm elevation in Ring 1 (left) and Ring 2 (right)

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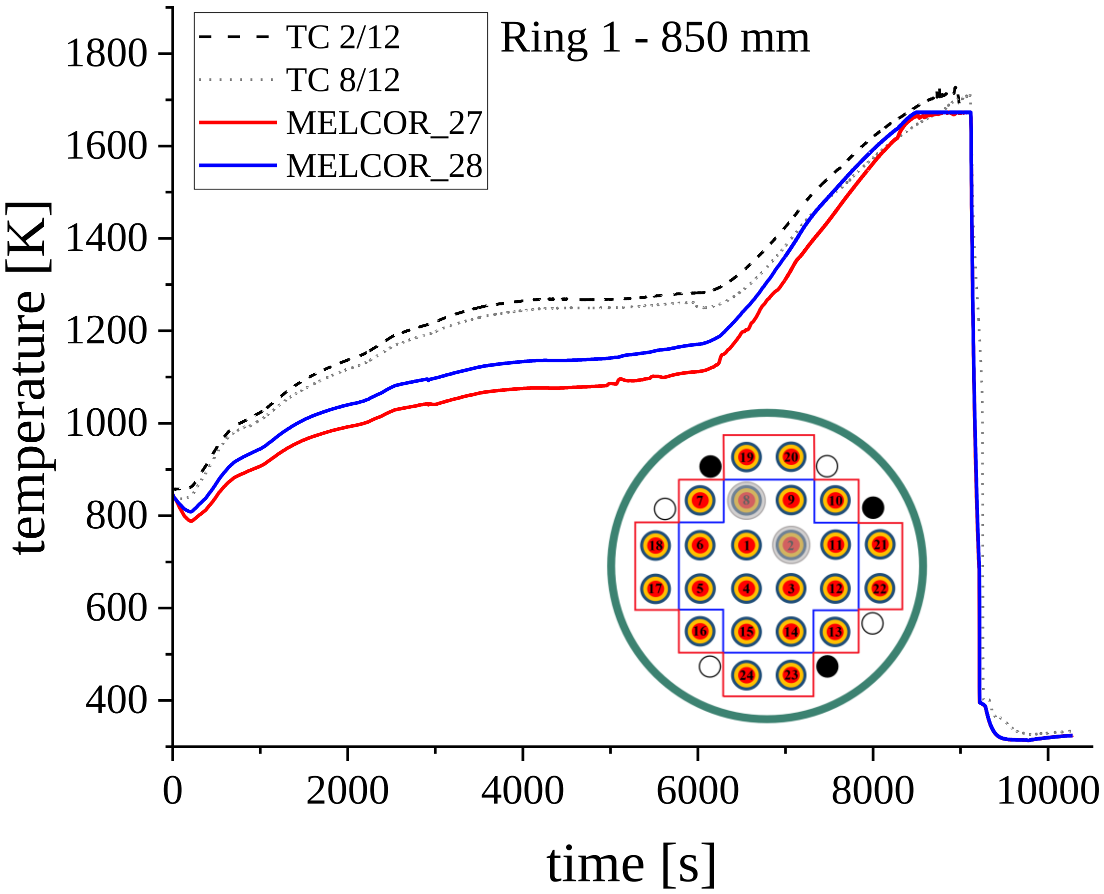
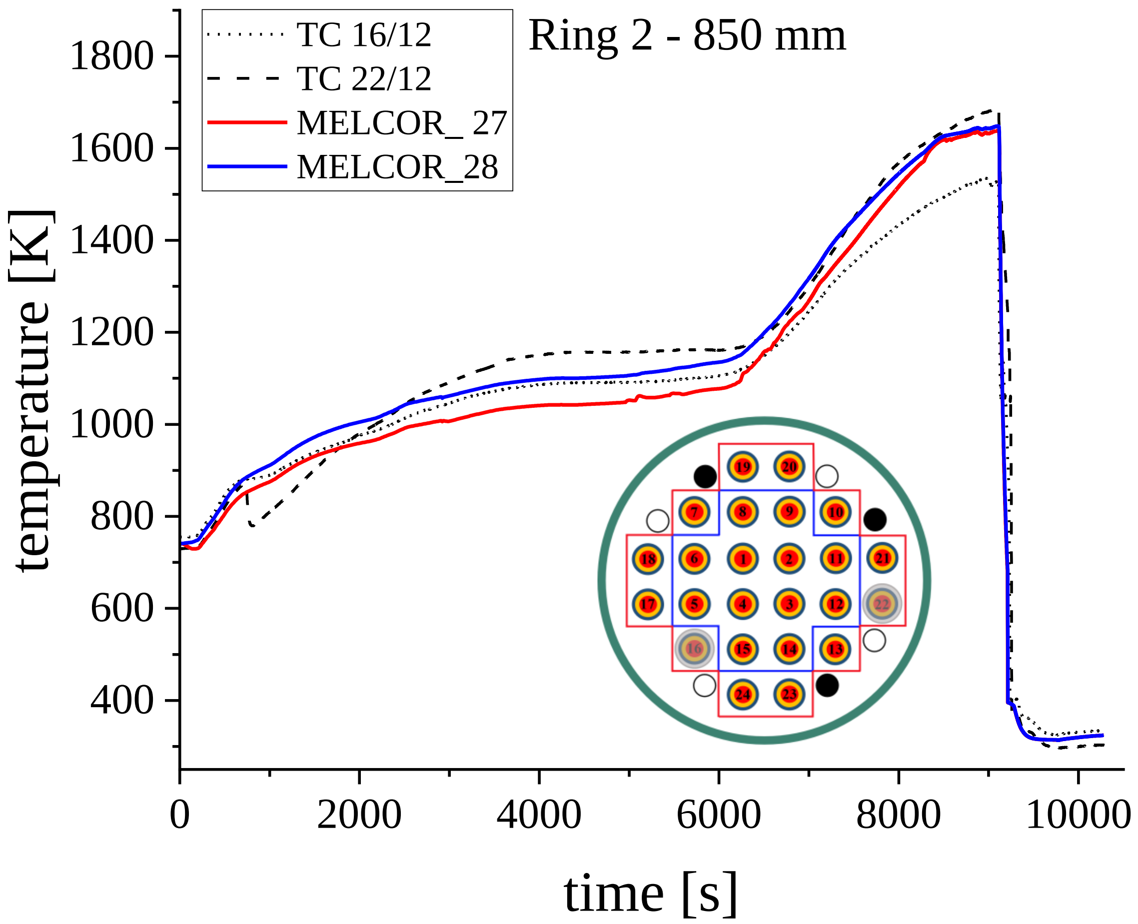
Simulation Results

Temperature Evolution – 850 mm elevation





(Cazado et al., 2026a)

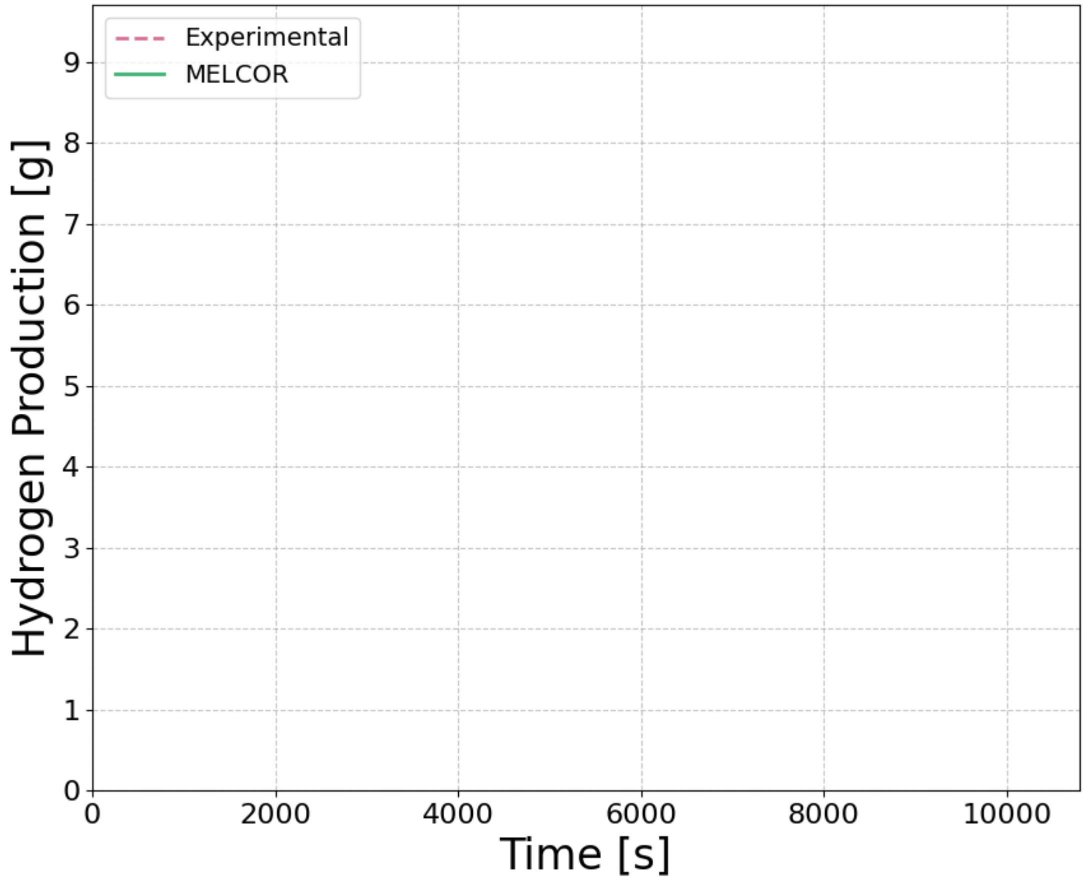
Cladding temperature at 850 mm elevation in Ring 1 (left) and Ring 2 (right)

Simulation Results

Hydrogen Evolution

It is estimatated, exp. that a total of ~2 g of H_2 come from the SS oxidation of the thermocouples‘ sheaths.
For FeCrAl → ~22% Total H_2
For ZIRLO → ~4% Total H_2

Those components are not modelled in MELCOR, but their effect are calculated based on the simulated temperatures and estimated exposed areas.



Cumulative Hydrogen production: Simulations (with SS oxidation effect) vs Exp. (Stuckert, 2022)

(Cazado et al., 2026a)

Simulation Results

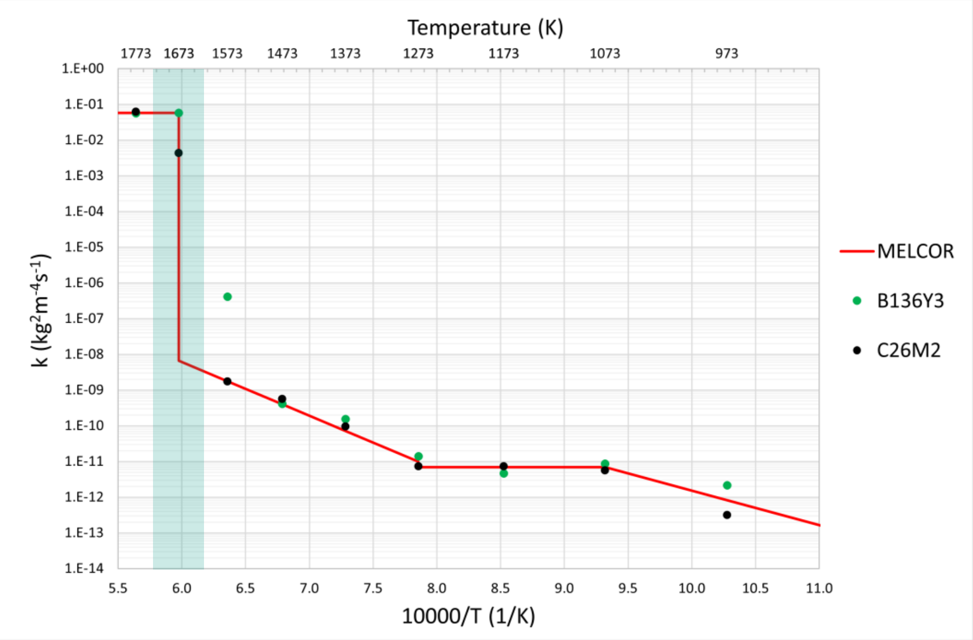
Evaluation of Uncertainties in Oxidation Kinetics

- Assess the impact of oxidation correlation uncertainties on hydrogen generation.
- Parameters studied:

  - **TSWITSCH**: 1673 ± 50 K ←Transition temperature from θ-Al_2O_3 to Iron-oxide kinetics.

  - **F_{AGAIN}**: [0.85, 1.15]
- **Uniform** probability distribution applied to both parameters
- **Random** sampling for 100 simulations.
- FoM: **Total H_2 production**

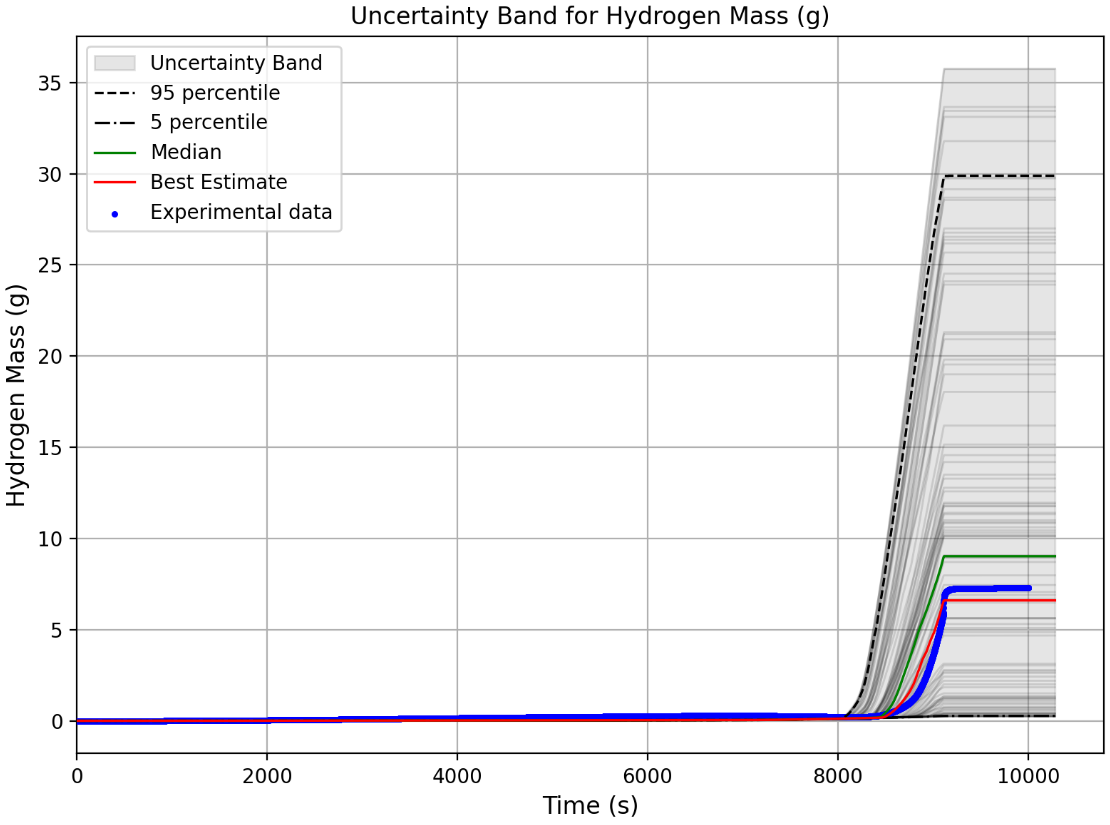
$$k(T) = F_A \cdot A_{gain} e^{\left(-\frac{B_{gain}}{T}\right)}$$



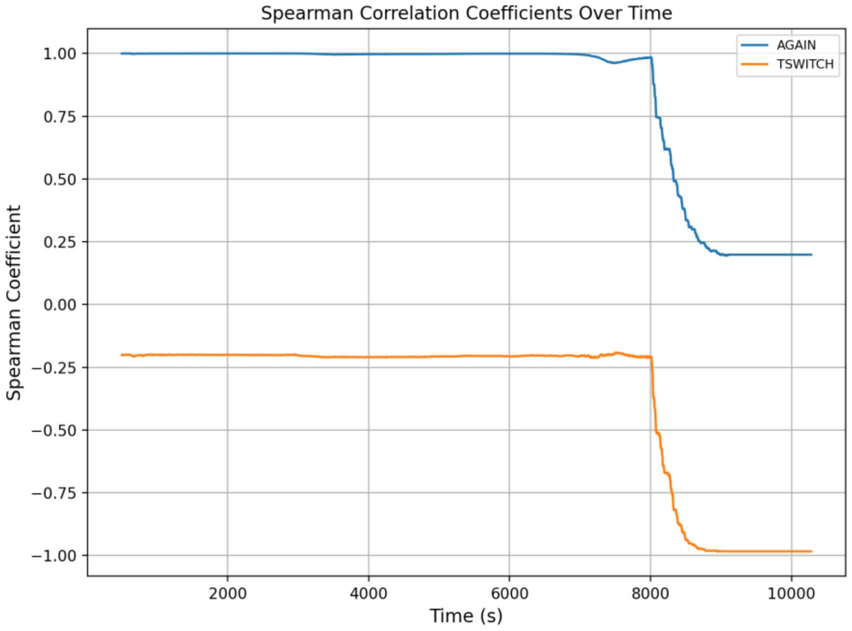
(Cazado et al., 2026a)

Simulation Results

Evaluation of Uncertainties in Oxidation Kinetics



- Both parameters influence H2 production but at different stages of the simulation.
- Primery driver: TSWITCH has a more significant impact on the final hydrogn production.



(Cazado et al., 2026a)

Simulation Results

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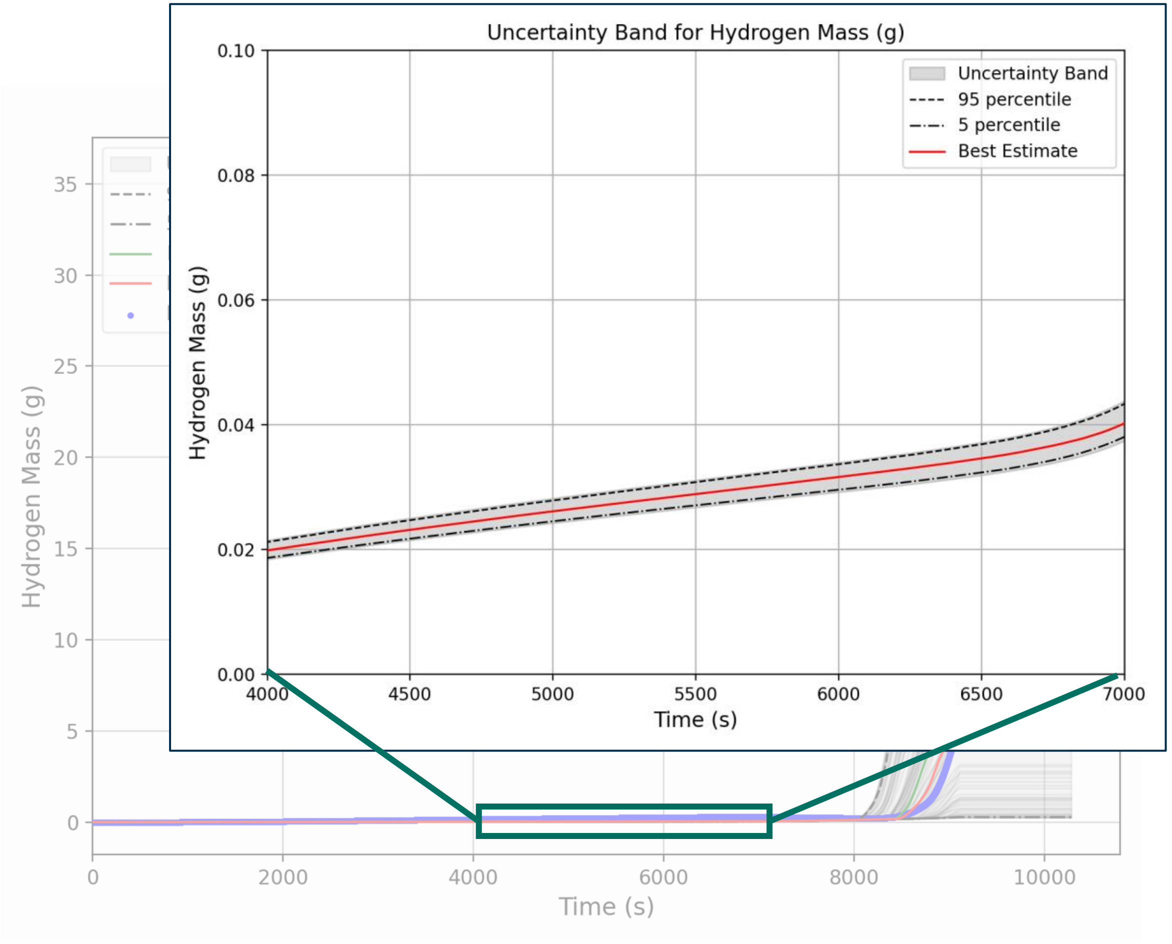

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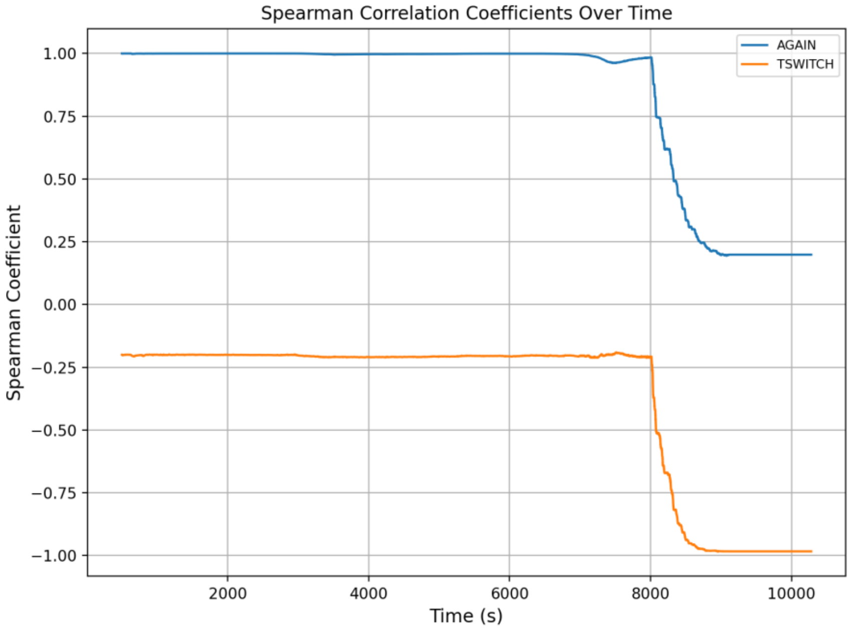

(Cazado et al., 2026a)

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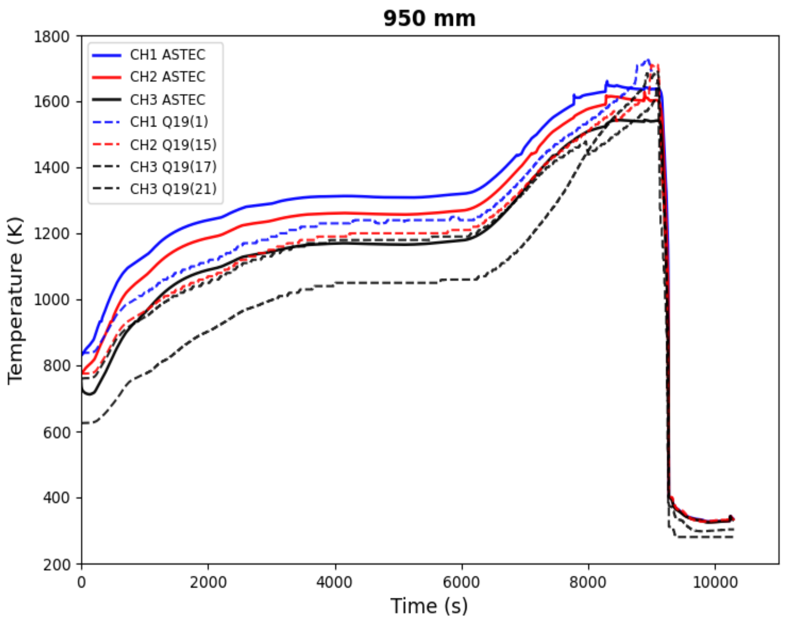
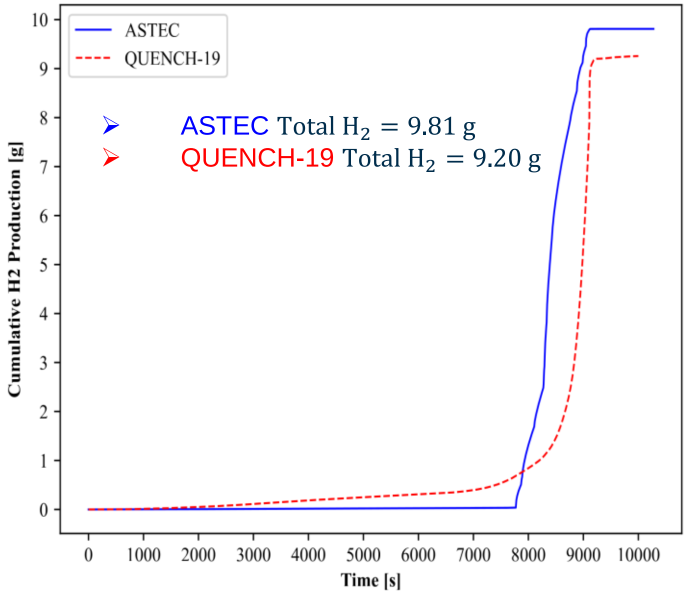
Other ATF-Related Activities

FeCrAl oxidation model development in ASTEC (Jimenez-Balbuena et al., 2026)

- New FeCrAl oxidation model developed by KIT in ASTEC with ASNR support.
- KIT single-effect tests provided the basis for dedicated FeCrAl oxidation modelling.
- Two oxidation regimes are represented: Al oxidation for protective Al_2O_3 formation up to ~1600 K, and Fe oxidation at higher temperatures.
- The model was validated against experimental data of the QUENCH-19 bundle test



Axial Cladding Temperature Evolution at 950 mm: Simulation–Experiment Comparison



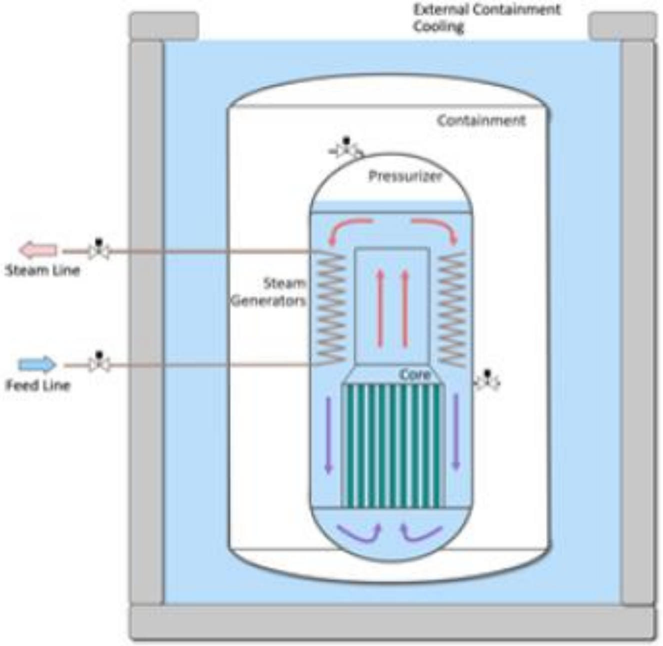
Total hydrogen release ASTEC vs. Experiment

Other ATF-Related Activities

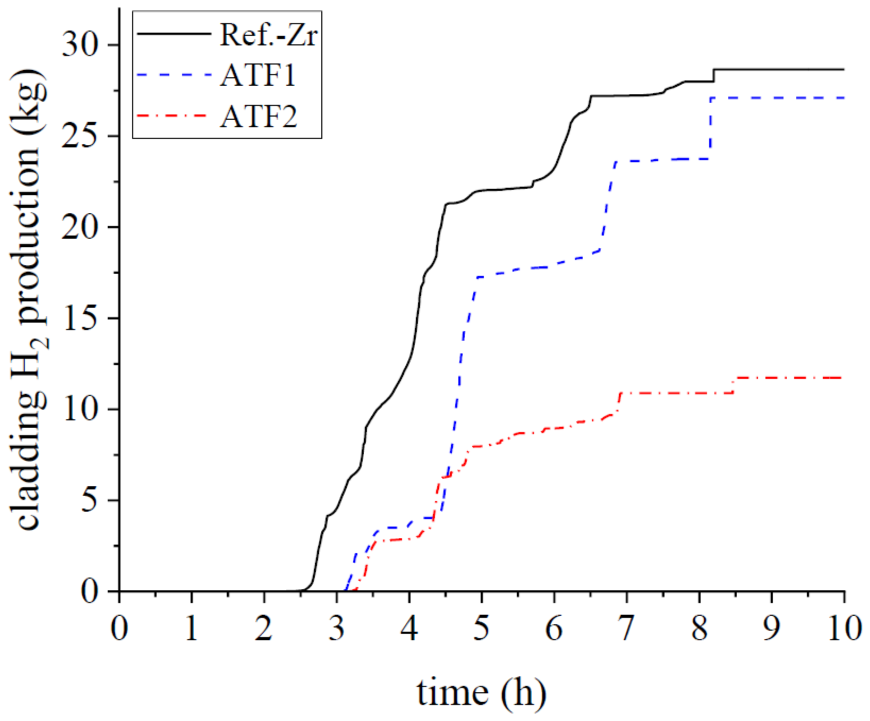
ATF Activity in SASPAM-SA Project

ASTEC code assessment of FeCrAl vs. Zircaloy in-vessel behavior

iPWR ~60 MWe
Submerged Containment



SA-1: 100% break on the CVCS makeup line (high elevation to avoid reverse flow)



(Cazado et al., 2026b)

ATF1 – FeCrAl oxidation kinetics

ATF2 – FeCrAl oxidation kinetics + FeCrAl properties

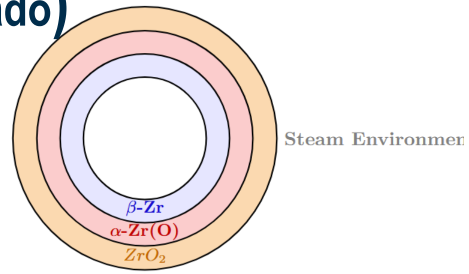
- FeCrAl had limited impact on key thermal-hydraulic variables.
- The implementations captured key FeCrAl benefits: reduced H_2 production and delayed rapid temperature rise before failure.
- Dedicated FeCrAl late-degradation models are still required for further assessments.

Other ATF-Related Activities

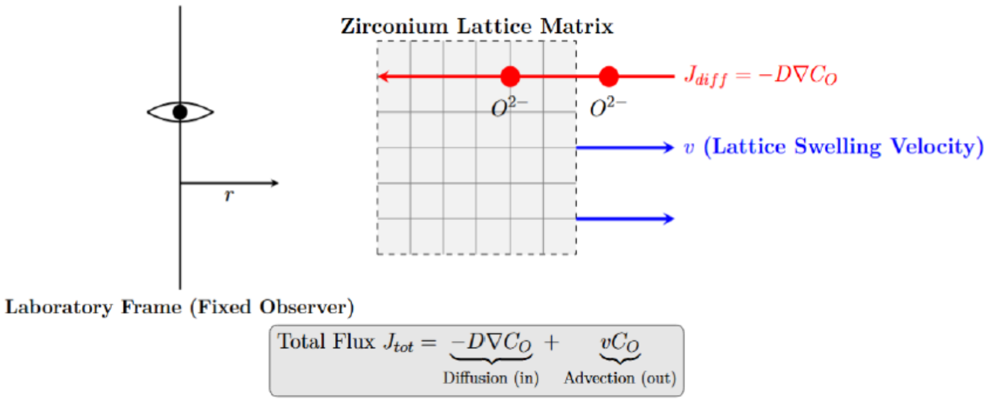
Development of a Moving Boundary Solver for Zr Claddings (L. Metay Peault & M.E. Cazado)

Under Development for Cr-coated Zr Claddings

- 1D cylindrical cladding.
- Formation of phases: α-Zr, β-Zr and ZrO_2
- Axial diffusion is neglected.
- Solver based on the Finite Volume Method.
- Moving Boundaries handled by the Arbitrary Lagrangian-Eulerian Method.
- Adaptative time step.



Cross-sectional scheme view of the concentric phases formed during Zr oxidation.

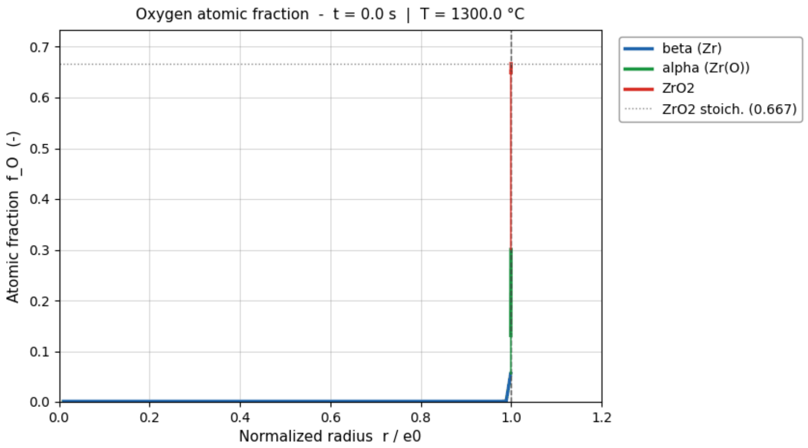


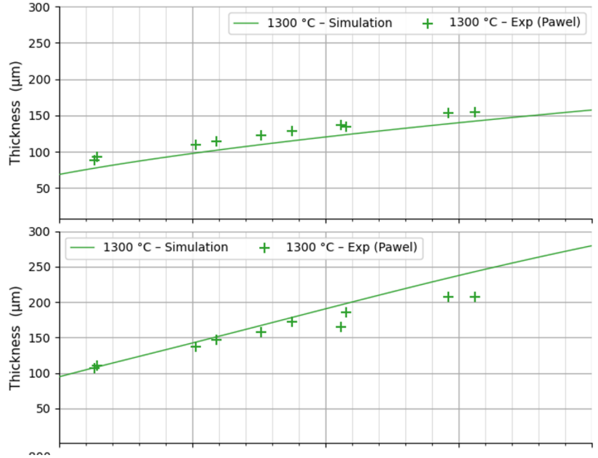
Mass conservation of oxygen, for a given phase “k” :

$$\frac{\partial C_{O,k}}{\partial t} + \underbrace{\frac{1}{r}\frac{\partial}{\partial r}\left(rvC_{O,k}\right)}_{\text{Expansion/contraction of the lattice}} = \underbrace{\frac{1}{r}\frac{\partial}{\partial r}\left(rD_k(T)\frac{\partial C_{O,k}}{\partial r}\right)}_{\text{Diffusion of oxygen}}$$

Mass conservation of Zr, for a given phase “k” :

$$\frac{\partial C_{Zr,k}}{\partial t} + \underbrace{\frac{1}{r}\frac{\partial}{\partial r}\left(rvC_{Zr,k}\right)}_{\text{Expansion/contraction of the lattice}} = 0$$





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Conclusions

- A MELCOR input deck for QUENCH-19 was developed following KIT report specifications and data obtained from the FeCrAl SETs at KIT.
- Although deviations were observed, MELCOR demonstrates good agreement with QUENCH-19 experimental data in terms of temperature evolution and hydrogen generation. Significant hydrogen generation mitigation below ~1400°C when compared to equivalent test performed with Zr-based alloys.
- Stainless steel oxidation from thermocouple sheaths has an important impact in ATF configurations.
- A preliminary U&SA was performed on two parameters affecting the oxidation correlation. Results indicate that the TSWITCH parameter has the strongest influence on hydrogen generation.
- Further work is under evaluation for including the oxidation of the thermocouples sheaths in the input deck model and increase the UQ parameters.

Conclusions

- KIT is involved in several ATF-related activities that includes: the development of FeCrAl oxidation modelling in ASTEC, SMR severe accident analyses with ATF cladding, and moving-boundary oxidation models for Zr/Cr-coated Zr.
- KIT aims to connect detailed material modelling with integral SA analysis. The standalone models developed at KIT can provide the physical basis needed to formulate, improve and validate advanced material models in integral SA codes.
- In addition, KIT has been contributed to different international projects related to ATF: OECD/NEA QUENCH-ATF, CRODODOX, ATF-TS, among others.

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Thank you for your attention

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