Experimental and Computational Activities on ATFs at KIT and GRS

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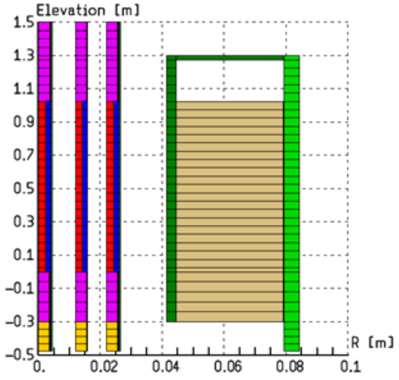


ATF cladding research at KIT and GRS

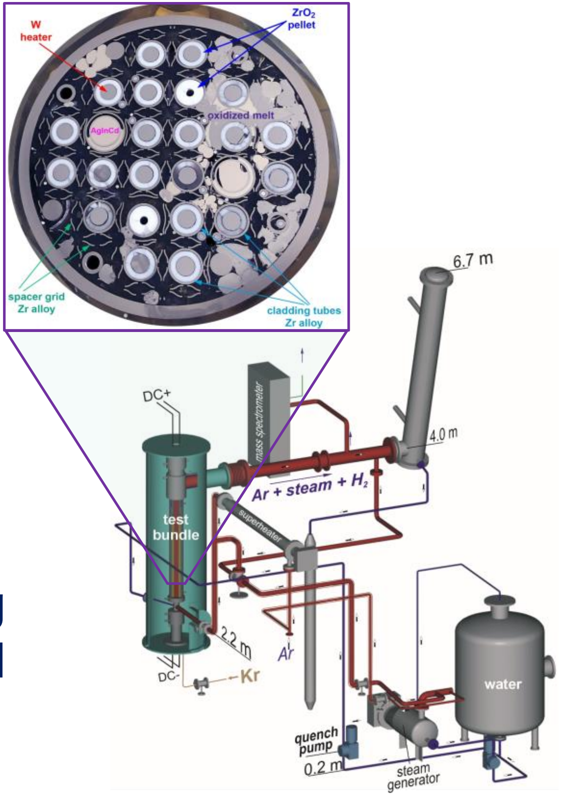
- Focused on HT behaviour of promising cladding materials
- Separate-effects tests and bundle experiments
- Model development, code validation, and code application (also GRS)
- Embedded in international cooperation programs
- and further international collaboration, e.g., with Westinghouse (USA) and SNU (South Korea)

The QUENCH/LICAS Facility

- **Unique large-test facility worldwide** for investigating the materials' behaviour in conditions representative of

- **Design basis accidents** (T ≤ 1200 °C)
- **Beyond design basis accidents** (1200 °C < T < 2300 °C)
- **Dry storage** (T < 450 °C for many months)

- **Providing high quality reference data and advancing understanding of physics to the international community**



QUENCH Activities on ATF cladding materials

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- **Bundle tests** in the framework of OECD-NEA QUENCH-ATF
- **Single-rod** oxidation and quench tests of ATF cladding segment samples
- HT furnace tests with **small samples** in various atmospheres for analysis of oxidation kinetics and degradation mechanisms
- Tests on **all promising ATF cladding concepts**, included Cr-coated Zry, FeCrAl, and SiC-based composites
- **Data for model development, code validation, and code application**

International Programs

International collaborations on ATF cladding

- OECD-NEA Joint Undertaking QUENCH-ATF
- IAEA Coordinated Research Project ATF-TS
- EC Projects IL TROVATORE and SCORPION
  - KIT coordinates WPs on fuel-cladding interaction
  - SCORPION devoted to sophisticated SiC-based composites
- EC Project OFFER
  - KIT is proposer of the CODEX-ATF-AIR bundle test at EK Budapest

See also: Proc. of the 29th International QUENCH Workshop, Karlsruhe, Germany, November 19-21, 2024, https://doi.org/10.5445/IR/1000177365

OECD-NEA Joint Undertaking QUENCH-ATF

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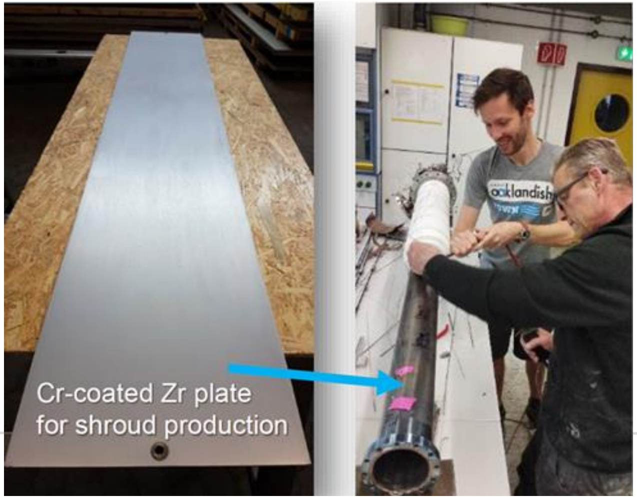
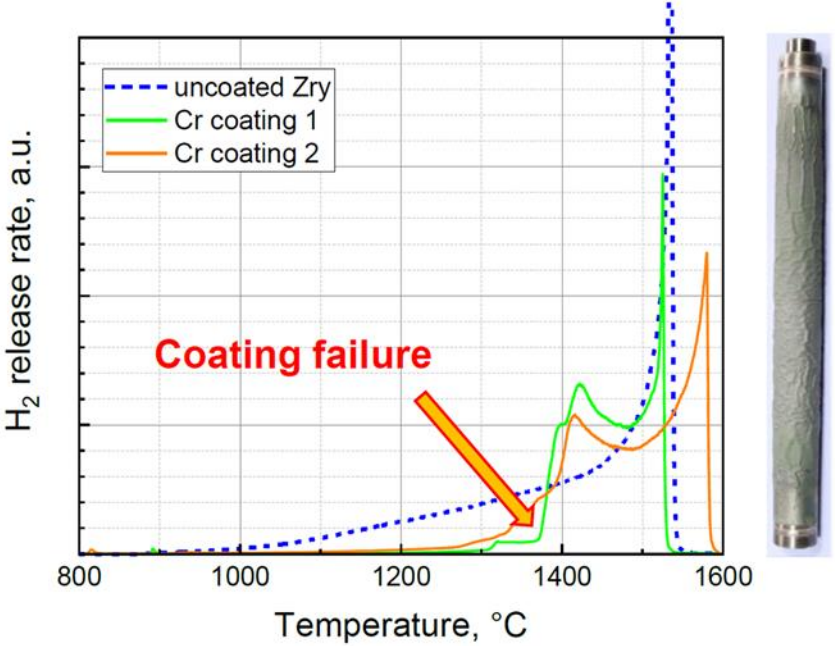
- KIT is Operating Agent
- Duration until October 2026
- Three QUENCH bundle experiments with **Cr-coated Zr alloy** cladding tubes
  - QUENCH-ATF 1: **Cold Spray Cr/ZIRLO** (Westinghouse) with **slightly beyond DBA** LOCA scenario (Tmax=1300°C) - **completed**
  - QUENCH-ATF 2: **Cold Spray Cr/ZIRLO** (Westinghouse) with **BDBA scenario** (Tmax=1600°C) - **completed**
  - QUENCH-ATF 3: **PVD Cr/ZIRLO** (WH/NNL) - **planned for summer 2025**
- **Benchmark exercises** for each test (coordinated by GRS)
- Extensive **post-test analyses** (KIT, ASNR) and **supporting SETs**
- **Phase II under discussion**

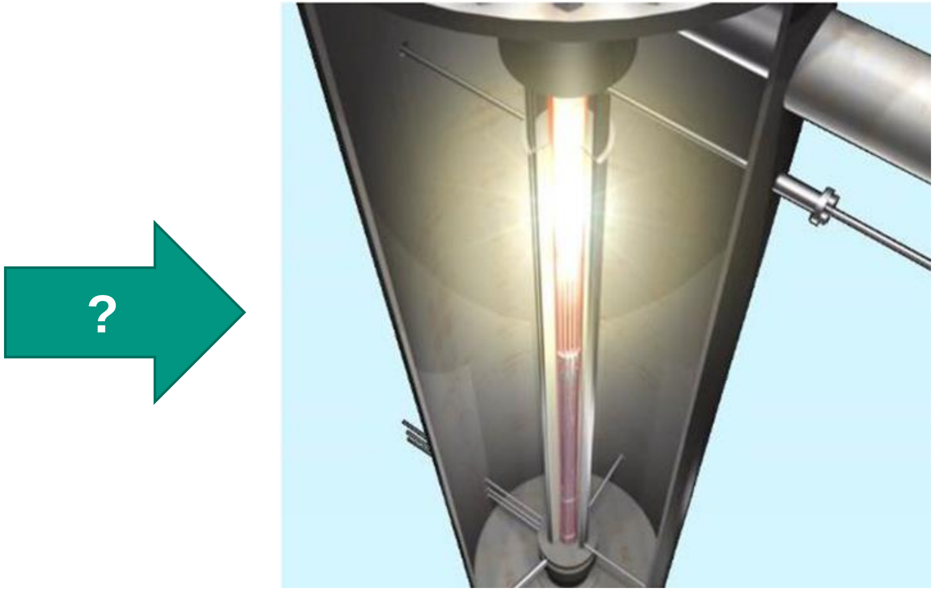
QUENCH-ATF 2 bundle experiment

- Conducted in August 2024
- SA test with **cold sprayed Cr-coated ZIRLO** cladding (Westinghouse) (24 rods, OD 9.144 mm)
- Max. temperature 1600 °C (significantly above the Zr-Cr eutectic temperature), then quenching phase
- Reference test QUENCH-15 with uncoated ZIRLO
- Two ATCRs with pellets of Eu_2O_3-HfO_2 from CRIEPI (Japan)
- Two rods pressurized similar to the QUENCH-18 bundle



Why QUENCH-ATF 2 test so exciting?





- **Single-rod** experiments with high heat losses → faster oxidation of coated samples after coating failure to Zry
- What happened under almost **adiabatic conditions** in the **bundle test**?

QUENCH-ATF 3 test scenario

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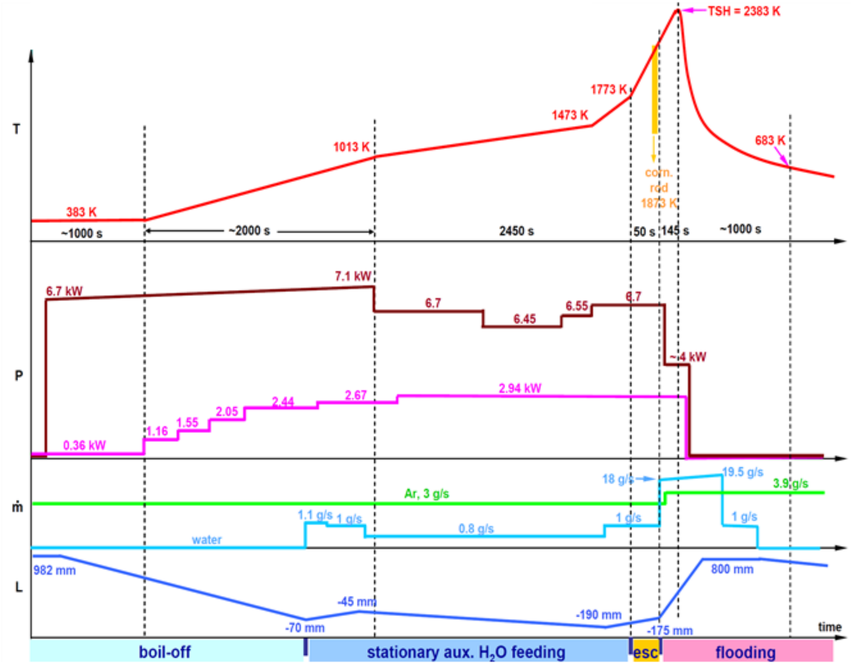
- The decision was taken for the scenario of the boil-off experiment QUENCH-11
- **Compromise between the options DBA and SA**
- Simulation of a depressurized plant sequence in which the core would be essentially dried-out
- Limited steam flow due to boiling of residual water
- The experiment QUENCH-11 was conducted in 2005, followed by a SARNET benchmark exercise with participants from **KIT**, **GRS**, INRNE, IBRAE, NRI, **RUB**, **IRSN** (now **ASNR)**, UZ, and INR

QUENCH-11 test scenario (Adapted for QUENCH-ATF3)

- **Water filling** of the bundle and heat-up to ~110°C
- **Boil-off** of the water-filled bundle to bundle foot accompanied by **bundle heat-up to ~1200°C**
- Continued boil-off with **enhanced bundle heat-up up to 1600°C** with water level kept close to bundle foot by injecting ~1 g/s of water
- **Quenching of the bundle** by a water flow of 50 g/s

QUENCH-11 test conduct (Zr)*



*Hering, W. and Groudev, P. and Heck, M. and Homann, C. and Schanz, G. and Sepold, L. and Stefanova, A. and Stegmaier, U. and Steinbrück, M. and Steiner, H. and Stuckert, J., (2007), Results of boil-off experiment QUENCH-11, https://doi.org/10.5445/IR/270068456

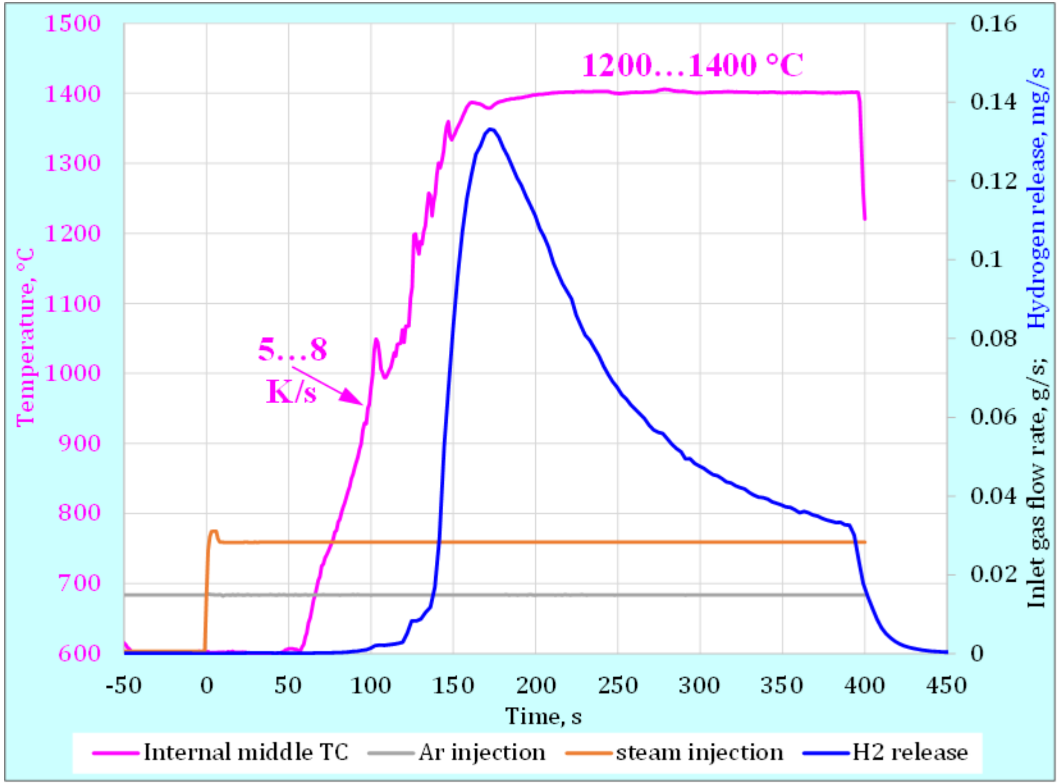
IAEA CRP ATF-TS

- KIT coordinates two work packages (Experiments, Benchmarks)
  - Various **separate-effects tests with Cr-coated cladding** at KIT

- Code benchmarking on bundle tests (fuel codes, SA codes)
  - **QUENCH-19**: <u>24-rods</u> bundle test with **FeCrAl** cladding (ORNL), **no pressurized rods**, quench with water
  - **DEGREE**: <u>9-rods</u> bundle tests with **PVD Cr/Zry cladding, pressurized rods**, cooling in Ar
  - **CODEX**: <u>7-rods</u> bundle test, **Cr coated opt. ZIRLO claddings (4 rods), pressurized rods**, quench with water

KIT - Transient tests in inductive furnace with Cr and CrN coated claddings: oxidation in steam

pre-test sample



post-test sample

BDBA conditions (max. surface T = 1400 °C) Hottest elevation @65 mm

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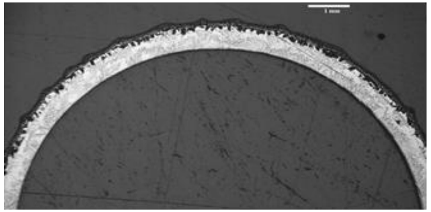
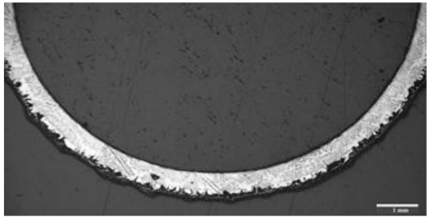
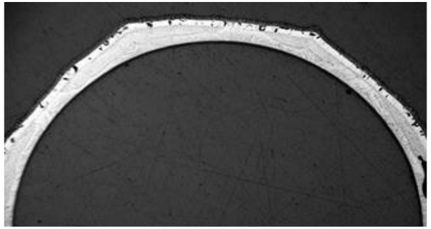
Initial 5 µm Cr layer



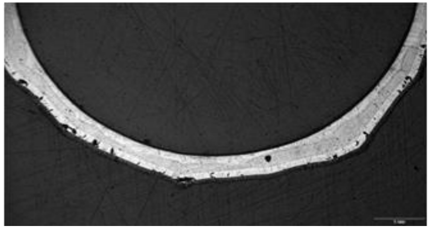
≈1.2 blisters per mm of circumference



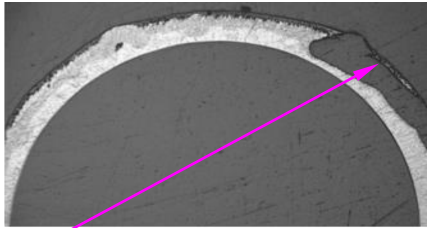
Initial 17 µm Cr layer



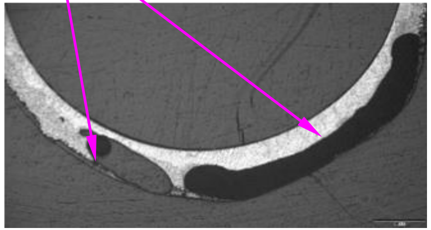
≈0.5 blisters per mm of circumference



Initial Cr (18 µm)/ CrN (8 µm) layers

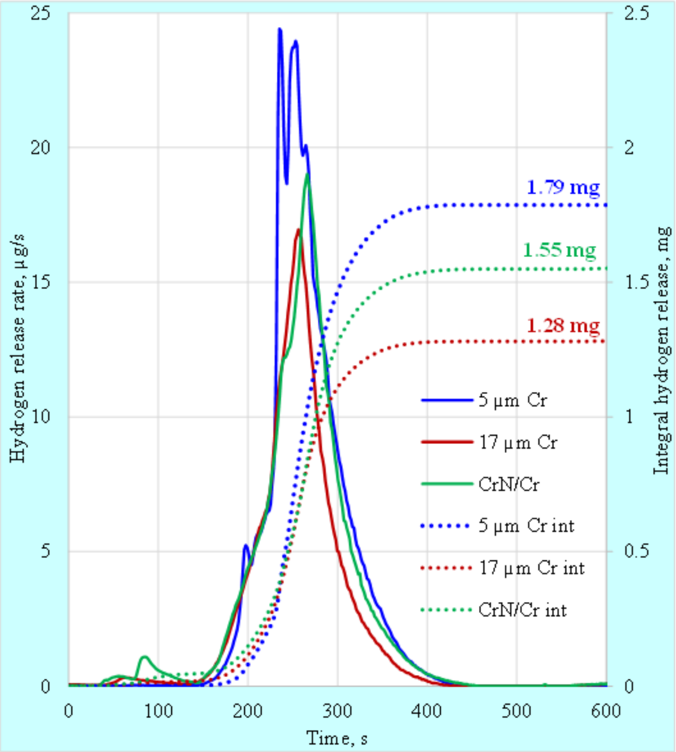


voids from (Zr, Cr) eutectic melt relocated downwards

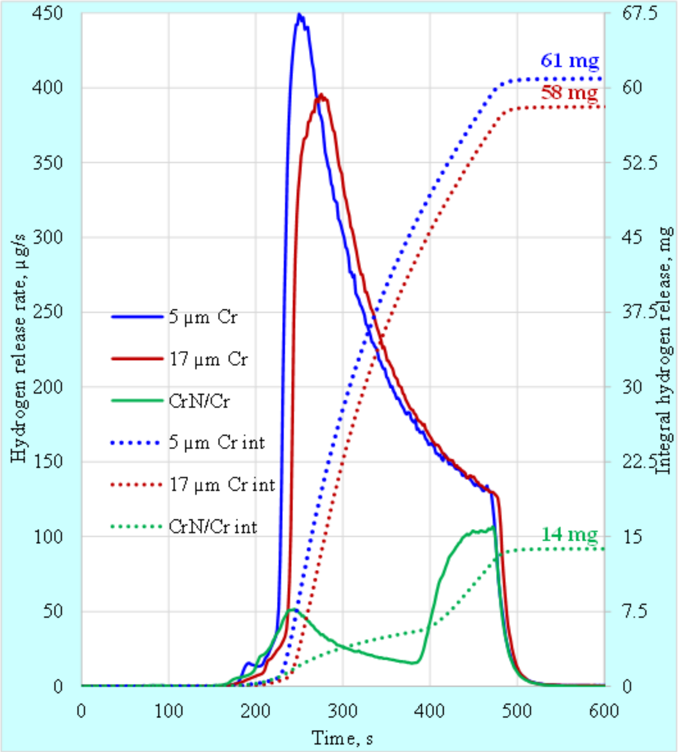


- Formation and relocation of (Zr,Cr) eutectic **melt** for Cr/CrN coating → perhaps due to the lack of intermediate oxidation of part of the Zr, which could not react with steam due to the barrier effect of CrN layer

Hydrogen Release

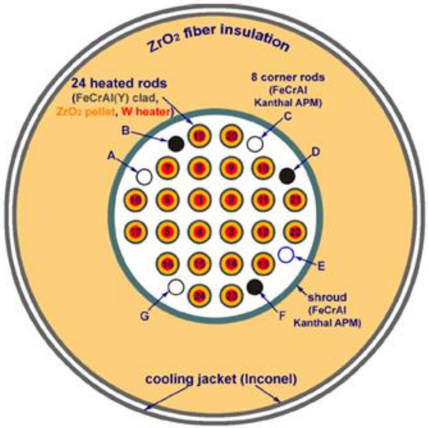


DBA (max. surf. **T = 1200 °C**)

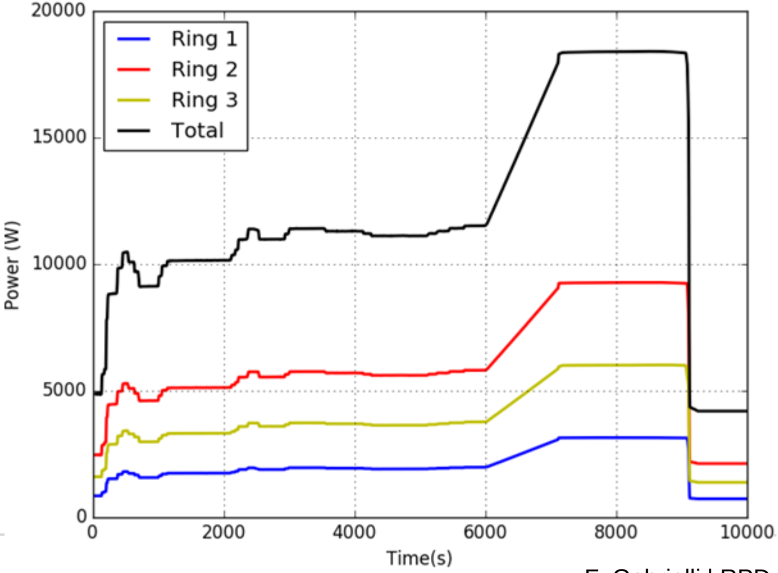


BDBA (max. surf. **T = 1400 °C**)

The QUENCH-19 Test

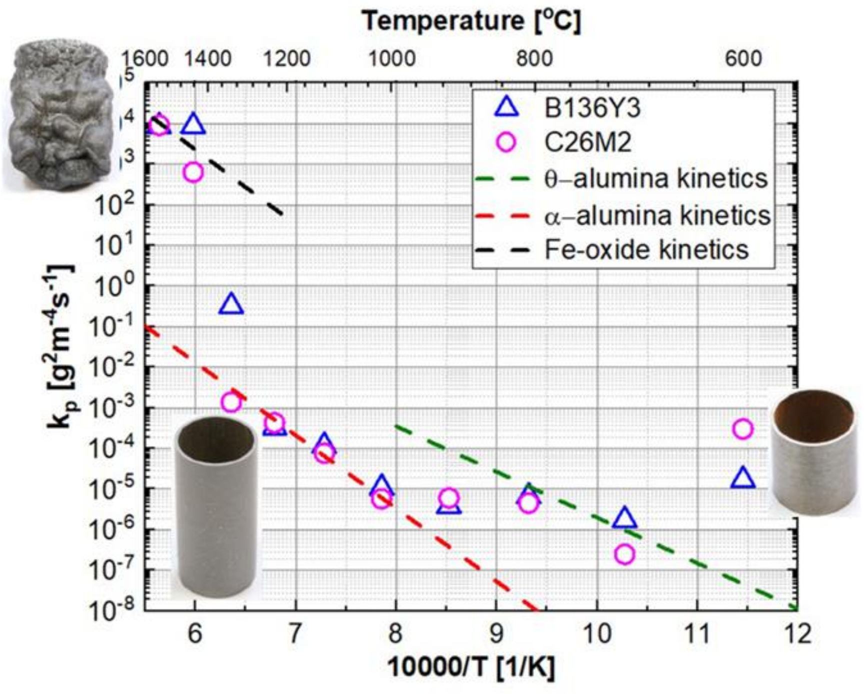


- Phase 1: heating up to ~600 °C (4 kW)
- Phase 2: power increase up to 11.5 kW (pre-oxidation)
- Phase 3: power increased up to 18.12 kW (5 W/s) (T_{pct}~1500 °C)
- Phase 4: power reduced to 4.1 kW



- Atmosphere of Ar (3.45 g/s) and superheated steam (3.6 g/s).
- Reflooding at ~9100 s
  - Fast initial injection of 4 kg of water
  - Slow injection 48 ~ g/s of water

Oxidation of Nuclear Grade FeCrAl Alloys



Steam oxidation kinetics of nuclear-grade FeCrAl alloys

- Three different correlations needed
- Fitting functions for weight gain provided by the QUENCH team to the ATF-TS

$$K = \begin{cases} 9.62 \times 10^{-12}\,[\mathrm{g^2/cm^4 s}], & T \leq 1473\ \mathrm{K} \\ A_B \exp\left(\dfrac{-E_B}{RT}\right), & 1473 < T < 1648\ \mathrm{K} \\ A_{Fe} \exp\left(\dfrac{-E_{Fe}}{RT}\right), & T \geq 1648\ \mathrm{K}\ (melting\ point\ of\ FeO) \end{cases}$$

A_B=3·10^9 g^2/cm^4 s **E_B=594354 J/mol**

A_{Fe}=2.4·10^6 g^2/cm^4 s **E_{Fe}=352513 J/mol**

C. Kim et al.: Oxidation mechanism and kinetics of nuclear-grade FeCrAl alloys in the temperature range of 500–1500 °C in steam, Journal of Nuclear Materials Volume 564,2022,153696, ISSN 0022-3115

IAEA CRP ATF-TS: Validation against QUENCH-19

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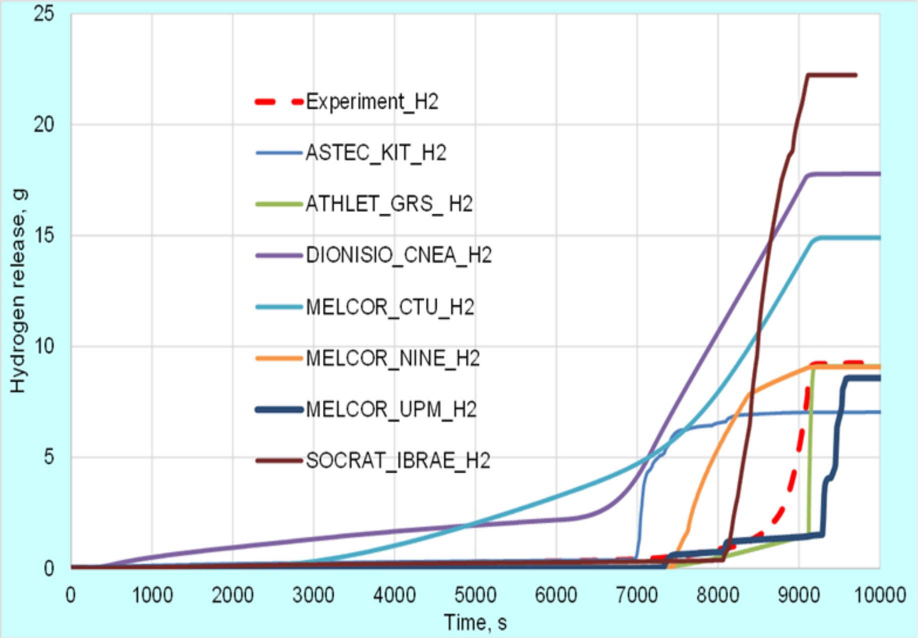
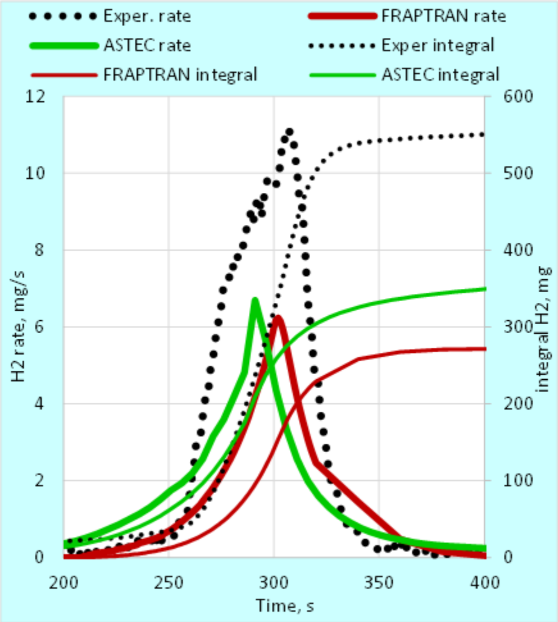


- ➢ Good prediction for the total mass of released hydrogen

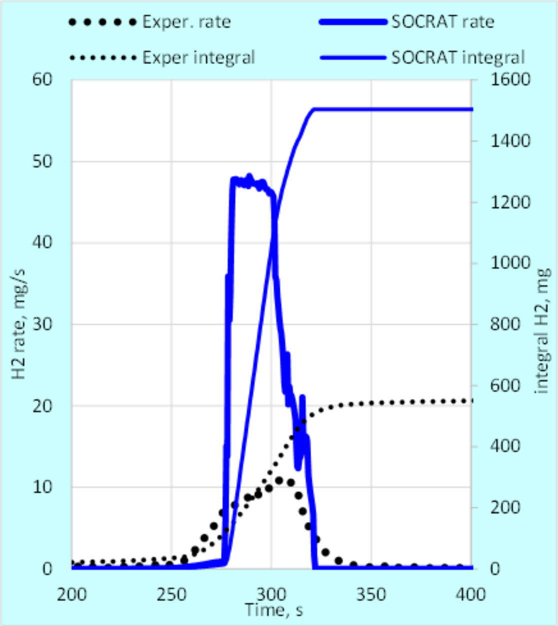
- ➢ Deviations due to either:
- ➢ increased calculated temperatures (overprediction of hydrogen)
- ➢ or individual modification of the Fe oxidation correlation

IAEA CRP ATF-TS: Validation against DEGREE-B3

ASTEC and FRAPTRAN (w/o Zr oxidation)

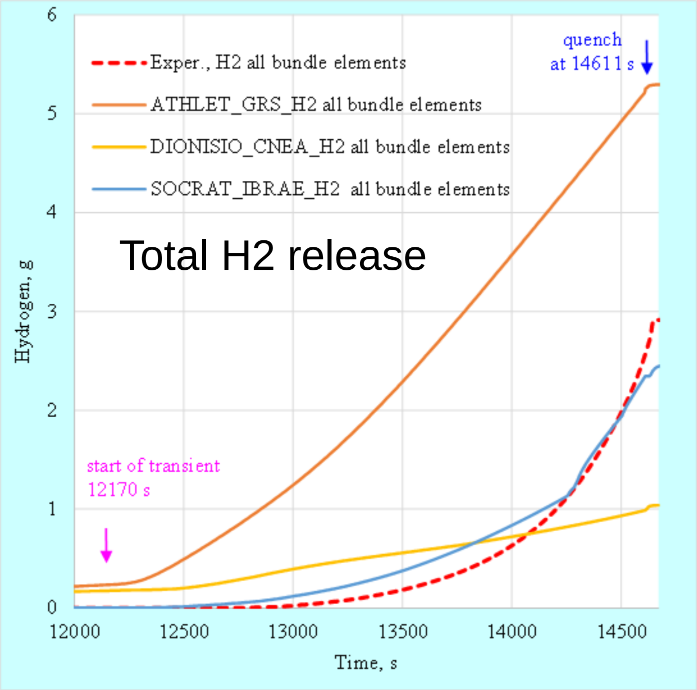


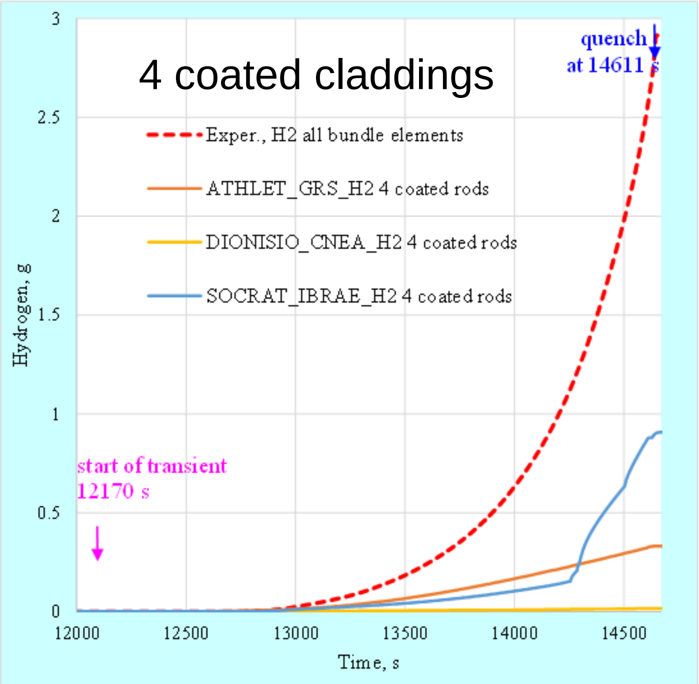
SOCRAT (with Zr oxidation)



- **Only the Cr oxidation** (ASTEC, FRAPTRAN) leads to an underestimation of hydrogen, while **inclusion of the Zr oxidation** too early (SOCRAT) gives an overestimated result

IAEA CRP ATF-TS: CODEX-ATF





ATHLET-CD: Temperature overestimation
SOCRAT: good prediction (accurate T, oxidation of Zr substrate under Cr layer)
DIONISIO: underestimation (shroud not simulated)

ATHLET-CD: oxidation of Zr substrate not simulated
SOCRAT: simulation of Zr substrate
DIONISIO: large T underestimation

Main outcomes of the IAEA ATF-TS Benchmarks

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- Good flexibility of the codes in adapting new materials
- Oxidation modules modified to take into account the correlations of FeCrAl and Cr oxidation
- Temperatures are mostly overestimated (before the escalation cases), whereas the hydrogen release values are widely scattered
- Further research is needed to take into account processes above the eutectic points

ATFs Model Development and Validation at KIT and GRS

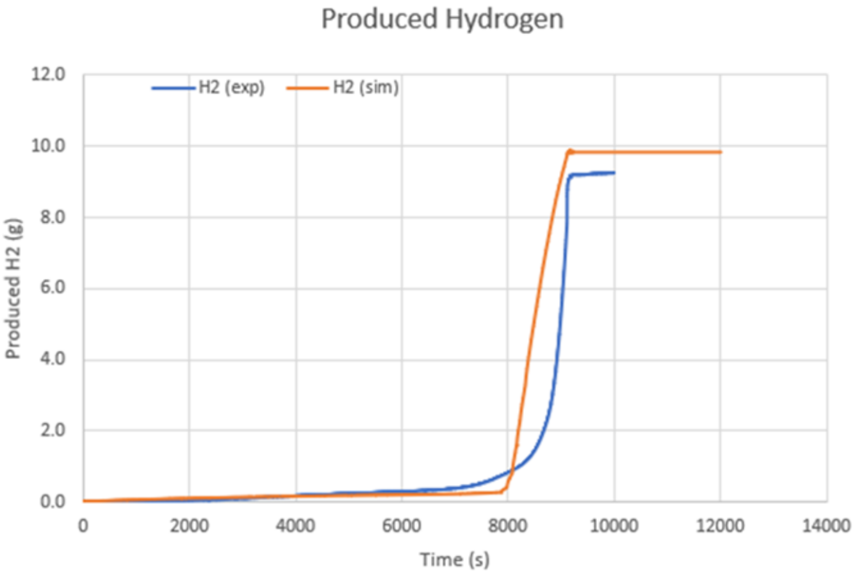
ATF simulation capabilities of AC^2

- AC^2 was optimized and developed for U-Zr systems
- Recent developments towards materials of:
  - FeCrAl (GRS)
  - Cr coated Zr (RUB)
- Effects of ATF in AC^2
  - **Simple material properties**
  - **Oxidation**
  - **Melt formation and relocation**
  - Ballooning / mechanical rod behaviour
  - Lower plenum phenomena
  - Burn-up / Fission product release

Main focus of development

AC²/ATHLET-CD: Analysis of the Q-19 test

- ➢ Slight overprediction of cumulated H2 production
- ➢ Small deviations in temperatures
- ➢ Steam starvation model needs update
- ➢ Correlations not fitting perfectly
- ➢ Transition ranges could be smoother



- ➢ Acceptable results, but further investigations on effects of FeCrAl on the accident evolution continue

AC²/ATHLET-CD
Cr-coated Zr Oxidation Model - CODEX-AIT-ATF

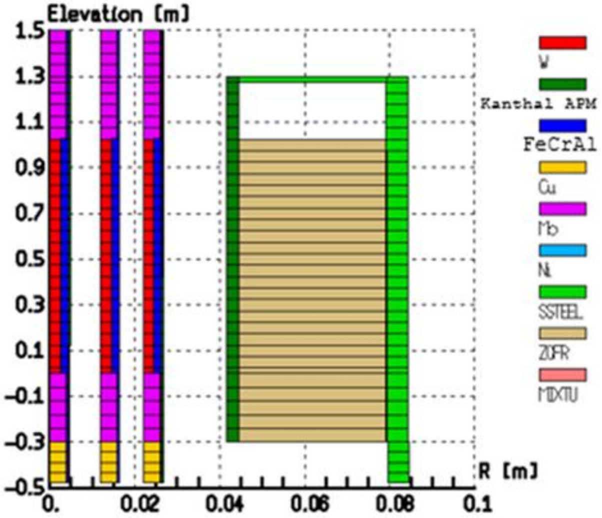
- Minor adjustments for air oxidation of Cr-coated Zr
- Mainly to do pre-and post-test calculations for CODEX-AIT-ATF experiment
- **Until Cr coating failure** (for steam AND air):

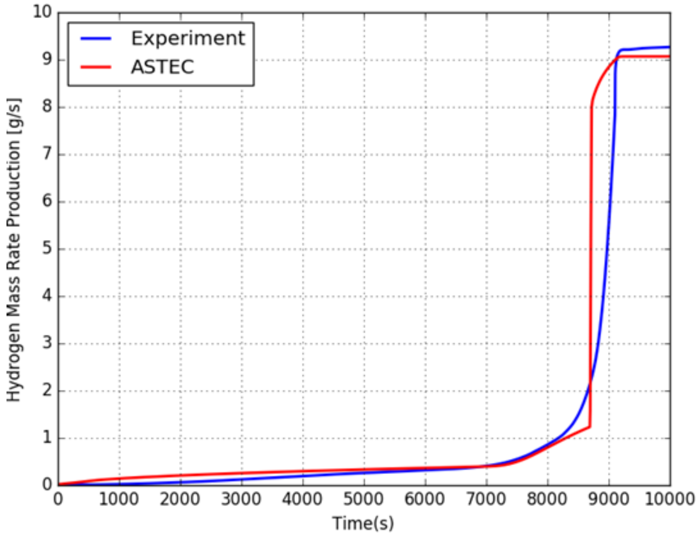
$$K = 207.1 \cdot \exp\left(\frac{-240000}{RT}\right) \quad \left[\frac{kg^2}{m^4 s}\right]$$

- Enthalpy of reaction changed, as well as amount of H2 produced (for steam)
- Cr coating is assumed to fail at T=1600 K
  - Failure mechanism not modelled in detail (yet)
- After failure, standard air and steam oxidation models are used

ASTEC: Analysis of the Q-19 test (2023)

- FeCrAl oxidation laws employed only instead of Zr material properties





- The final amount of H2 is reasonably well reproduced
- Behaviour below the eutectic formation (1550 K) temperature not well reproduced

Development of a FeCrAl Oxidation model in ASTEC

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- **KIT/ASNR shared activity** to improve the ASTEC modelling for FeCrAl cladding behaviour in steam environment at low and moderate temperatures
- Based on the QUENCH SETs, detailed oxidation kinetics considered

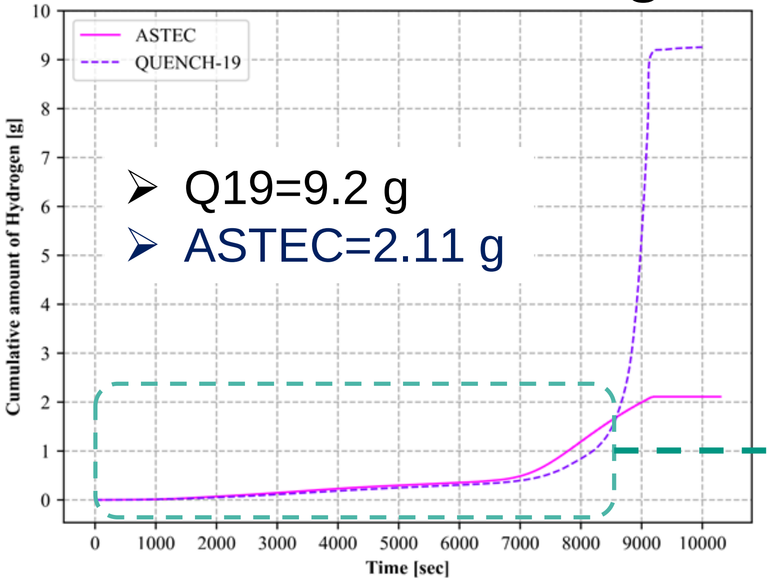
$873 < T < 1173$	$1173 \leq T \leq 1273$	$1273 < T < 1648$	$T \geq 1648$
Transient Alumina	Alumina	α-Alumina	FeO-Oxide

(Courtesy of Z. I. Jiménez)

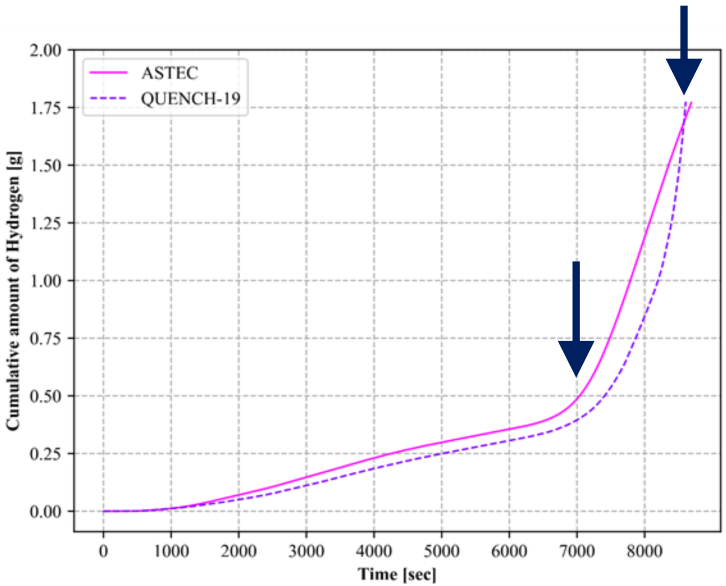
- …plus implementation of the physical models for the mass gain and thickness oxide layer evaluations, and the FeCrAl thermophysical properties
- **Model successfully validated against the QUENCH SETs**

Z. I. Jiménez, F. Gabrielli, M. E. Cazado, V.H. Sanchez-Espinoza, L. Laborde, L. Carenini, P. Drai, 2024, FeCrAl Oxidation Model Development on the ASTEC Code and Preliminary Validation Against QUENCH Experiments, Proc. Of the 29th International QUENCH Workshop, Karlsruhe, 19-21, November, https://doi.org/10.5445/IR/1000177365

ASTEC: Validation against Q-19



- Q19=9.2 g
- ASTEC=2.11 g



	T≈1550 K	T≈1612 K
ASTEC	0.49 g	1.77 g
Q19	0.4 g	1.77 g

- Model successfully validated in the expected range of temperature (up to 1550 K)

Z. I. Jiménez, F. Gabrielli, M. E. Cazado, V.H. Sanchez-Espinoza, L. Laborde, L. Carenini, P. Drai, 2024, FeCrAl Oxidation Model Development on the ASTEC Code and Preliminary Validation Against QUENCH Experiments, Proc. Of the 29th International QUENCH Workshop, Karlsruhe, 19-21, November, https://doi.org/10.5445/IR/1000177365

Codes' Validation: Conclusion and Outlook

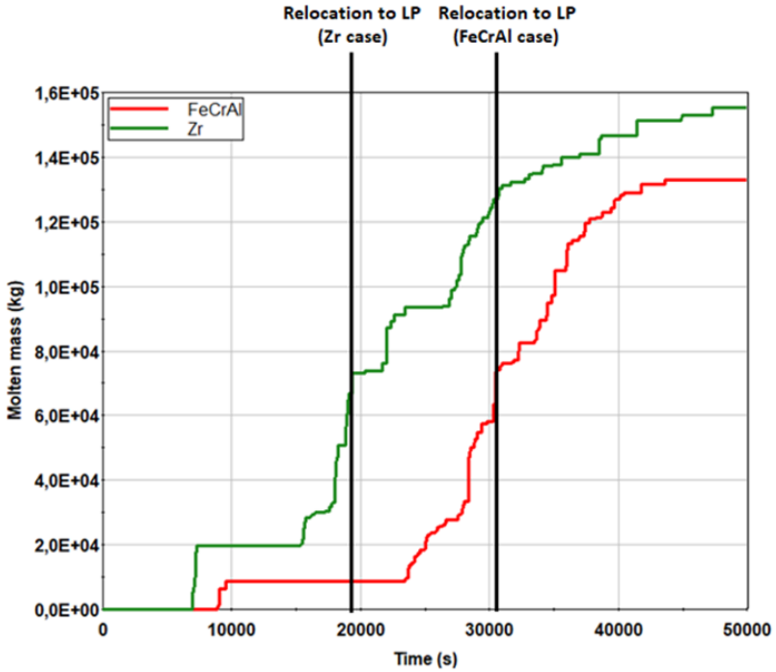
- **AC²/ATHLET-CD (GRS)**
  - FeCrAl and Cr-coated oxidation models developed and applied
  - Qualitatively good results, but additional efforts needed for ballooning, Cr-coating failure mechanism, oxidation models, FP release, further material interactions
- **KIT**
  - ASTEC validation against Cr-coated tests by KIT/ASNR (preliminary modelling approach by ASNR)
  - Development and validation of an advanced FeCrAl oxidation model in ASTEC (KIT/ASNR shared activity)
    - Further activity planned to extend the model for very high T conditions

Preliminary Plant Applications at KIT and GRS

Preliminary studies on the impact of ATF cladding materials on SA progression in NPPs

AC²/ATHLET-CD: UO2-FeCrAl interaction model

- Preliminary plant evaluations shown in CSARP2024
- Preliminary FeCrAl-UO2 interaction model implemented
  - Data from OECD-NEA TCOFF-2 project (still on-going)
- Amount of UO2 dissolved by FeCrAl
  - Calculations with NucleaToolbox (based on the NUCLEA database)
- Suggested models turn out to be valid

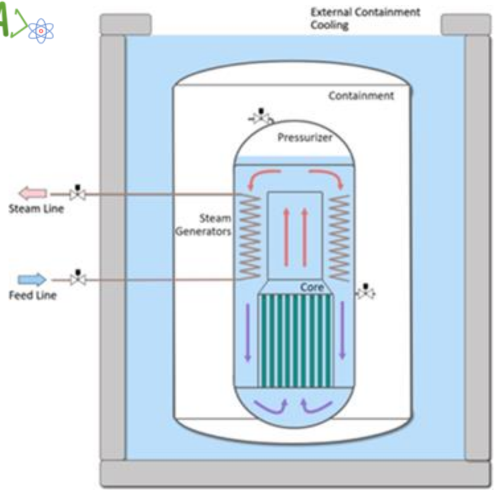


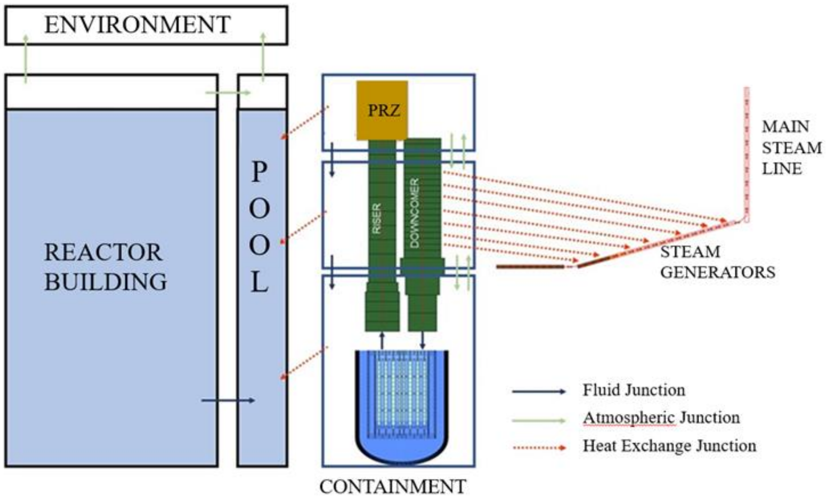
AC²/ATHLET-CD: UO_2-FeCrAl interaction model

- **ONLY** Oxidized FeCrAl (Fe) reacts with UO2
  - Dependent on the average oxidation state of cladding, different liquid fractions were obtained
  - Reaction almost instant

- Since extensive FeCrAl oxidation begins at around its liquification temperature → Competing phenomena: oxidation vs melt relocation
- Impact of the model limited when limited in-core damage
- Benefits are scenario dependent

ASTEC: postulated SA in a generic iPWR





- Generic iPWR Design-1 (Submerged containment, P~60 Mwe)
- ASTECv3.1.1 model developed in the framework of the SASPAM-SA project
- Comparing the effect of employing Zr, FeCrAl, and Cr-coated alloys in a postulated SA sequence on the cumulated H2 production

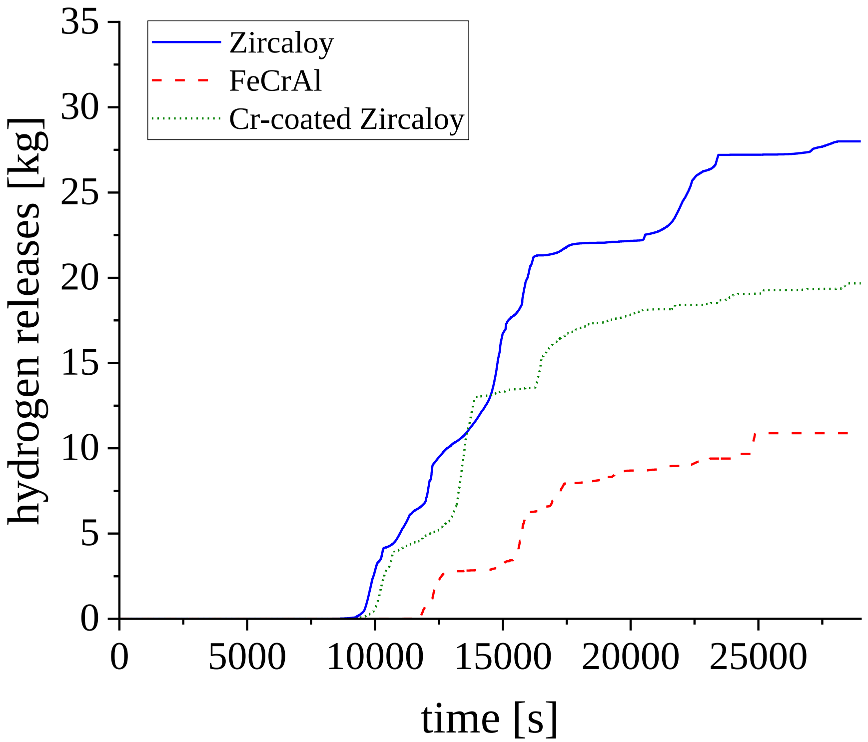
M.E. Cazado, et al. (2025), Impact of Advanced Technology Fuel Cladding Materials on the Progression of Severe Accidents in a Generic Natural-Circulation iPWR, Accepted Conference Paper, NURETH-21, August 31 – September 5, Busan, South Korea

ASTEC: postulated SA in a generic iPWR

- Goal: evaluating the effect on the H2 production → **Same geometrical model of the cladding regardless the alloy employed**
- Profiting of the ASTEC versatility, by modifying the existing structure of Zr-based alloy properties
- Thermophysical, thermodynamic, and oxidation correlations specific of FeCrAl and Cr-coated alloys
- Cr-Coated: once reached the eutectic T, Zr properties employed

M.E. Cazado, et al. (2025), Impact of Advanced Technology Fuel Cladding Materials on the Progression of Severe Accidents in a Generic Natural-Circulation iPWR, Accepted Conference Paper, NURETH-21, August 31 – September 5, Busan, South Korea

Results: H2 Production from the cladding



- FeCrAl offers more advantages the conditions predicted in the postulated scenario

- Reduction of the H2 to uncoated Zry, when considering only the cladding oxidation
  - **Cr-coated Zry ~30%**
  - **FeCrAl ~60%**

M.E. Cazado, et al. (2025), Impact of Advanced Technology Fuel Cladding Materials on the Progression of Severe Accidents in a Generic Natural-Circulation iPWR, Accepted Conference Paper, NURETH-21, August 31 – September 5, Busan, South Korea

Conclusion and Outlook

- KIT is contributing to worldwide research on ATF cladding mainly via international collaborations with the focus on testing at (very) high temperatures at the QUENCH facility

- **Experiments at KIT**
  - QUENCH-ATF 3 **PVD** **Cr/ZIRLO** (WH/NNL) based on QUENCH-11 **(Summer 2025)**
  - Behaviour of long-term ATF materials under DBA and BDBA conditions (QUENCH-ATF Phase II under discussion)

Conclusion and Outlook

- **Computational activities at GRS (AC^2/ATHLET-CD)**
  - Improvement/validation of FeCrAl (GRS) and Cr-coated (RUB) models
  - FeCrAl-UO2 interaction developed and under improvement
- **Computational activities at KIT (ASTEC, MELCOR)**
  - ASTEC: advanced FeCrAl and Cr-coated models developed, validated, and continuously under improvement (**KIT/ASNR shared activity**)
  - ASTEC: applications to SMR and generic BWR Mark-I *
  - MELCOR: validation against Q-19 + U&Sa *
- **KIT-GRS Cooperation on AC^2**
  - Focus on: Fuel fragmentation after quenching, AI, AC^2 validation, …

*EU SEAKNOT mobility program

BOOK-THE-DATE!

30^{th} International QUENCH Workshop

Karlsruhe Institute of Technology,

Karlsruhe, Germany

December 16-18, 2025