

APPLICATION OF AC²/ATHLET-CD AND ASTEC FOR ATF EXPERIMENTS IN THE FRAME OF ONGOING INTERNATIONAL PROJECTS

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Outline

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- Modelling Approach
 - Correlation
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- Experiment and Simulation Results
 - QUENCH-15 (AC² and ASTEC)
 - QUENCH-03 (AC²)
- Conclusions



Motivation and Background

- The investigation of ATF (Accident Tolerant Fuels) materials had already started before the accident at the Fukushima Daiichi plant in 2011.
- A main objective for new ATF cladding materials is a significantly reduced kinetics of steam oxidation, which is accompanied by slower heating and therefore a longer time period before temperatures reach the melting point compared to zirconium-based cladding currently used in LWRs.
- Two options are currently under investigation with a certain TRL:
 - FeCrAI: at 1200°C, based on the composition the oxidation rate of FeCrAI could about a factor of 1000 lower than for zirconium. A slower reaction of FeCrAI with steam therefore reduces the rate of hydrogen generation, slowing down the pressure build-up in the pressure vessel and delaying the onset of hydrogen release into the containment.
 - Cr-coated optimised Zirlo: much slower oxidation than uncoated claddings, but once the protective state of the Cr-coating is lost at app. 1330 °C the oxidation of pure Zr at high temperatures occurs, leading to a potential escalation.
- Experimental and analytical projects are performed in the frame of IAEA and OECD
- Additionally, the modelling capabilities of severe accident codes were extended to be able to consider ATF. These new models need to be validated.



Current international projects for ATF

OECD QUENCH-ATF

The OECD/NEA QUENCH-ATF project was launched in 2021 to investigate the bundle behavior under DBA/DBC or DEC/BDBA/SA in three tests at the QUENCH facility at KIT

- Optimised Zirlo with Cr-coating: LOCA conditions,
- Optimised Zirlo with Cr-coating: BDBA conditions,
- Optimised Zirlo with Cr-coating or SiCf-SiC cladding tubes (to be decided)
- IAEA CRP ATF-TS (Testing and Simulation for Advanced Technology and Accident Tolerant Fuels)

Experimental and modelling activities for Cr-coated claddings and FeCrAl under DBA and DEC conditions

- Separate Effect Tests
- Bundle Tests like
 - QUENCH-19
 - CODEX-ATF-1



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Current Status of ATF Modelling in AC²/ATHLET-CD and ASTEC

- AC² and ASTEC are both able to predict the cladding behaviour of ATF namely FeCrAl and Cr-coating.
- In AC²/ATHLET-CD the oxidation models for FeCrAI and Cr-coatings are directly implemented in the code.
- In ASTEC there is the possibility to implement the data for oxidation and layer thickness growth directly in the input deck by the user.





QUENCH-19



Bundle Configuration

- Performed at KIT 2018
- FeCrAI claddings to investigate the cladding material behavior under SA conditions
- Scenario: similar to QUENCH-15 with Zirlo cladding
 - same bundle geometry
 - same electrical power input
- Bundle configuration made of different FeCrAI
 - alloys with slightly different compositions (see right):
 - 24 heated rods with tungsten heater and ZrO₂ pellet
 - 8 corner rods
 - 5 spacer grid
 - Shroud





Test Conduct

- Pre-Oxidation Phase 0 6020 s
- Transient Phase
- Quench Phase



Source: KIT



Simulation Results – Cladding Temperatures at 950 mm



- The deviations to the measured cladding temperatures could be reduced due to model improvement.
- But there is still an overestimation at the highest heated elevation.
- A peak is predicted for ASTEC, while AC²/ATHLET-CD predicts no peak in contrast to the experiment.



Simulation Results – Hydrogen Generation



 The oxidation behaviour is in better agreement to the experiment due to the model improvement.

 For AC²/ATHLET-CD especially by implementing the model directly in the code which allows a nodewise prediction instead of a global as in 2022 simulations.



CODEX-ATF1



Bundle Configuration

- Performed at EK HUN 2023
- 7-rod test bundle
- For the test CODEX-ATF1 two different types of claddings are implemented:
 - four Cr-coated optimised Zirlo claddings and
 - three uncoated optimized Zirlo claddings, which are located in the outer section with an angle of 120°.
- The rods are electrically heated by an u-shape wire.
- Zr2.5%Nb shroud insulated on the outer side.





Proposed Test Conduct

- The proposed scenario within CRP ATF-TS should focus on the following phenomena:
 - Ballooning and burst,
 - Oxidation of cladding external surface in high temperature steam,
 - Oxidation of inner cladding surface and secondary hydriding after burst,
 - Eutectic formation between Zr-Cr above 1300 °C.

Phase	Number of scenarios		Power	Argon	Steam/water
	NUBIKI	Original	(**)	(g/s)	(9/3)
Prepatory	0 - 1500	0 - 1500	600	0.2	0 - 0.2
			(400, AC ²)		
Heat-up I	1500 - 2300	1500 - 2000	1000	0.2	0.2
Heat-up II	2300 - 2500	2000 - 3000	2000	0.2	0.2
Quench	2500 - 4000	3000 - 4000	0	0.0	10.0

 Oxidation options in simulations

Scenario BIC

Name	Cr oxidation (ECORE)	Zr oxidation (HECU)
NUBIKI	Brachet (Cr only)	Cathcart Prater/Courtright
Original	Brachet (Cr only)	Cathcart Prater/Courtright
Escalation	Stahlberg with Cathcart Prater/Courtright >1300°C	Cathcart Prater/Courtright

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Simulation Results – Cladding Temperatures at 550 mm



- For the NUBIKI scenario, due to the shorter period of heat-up and power increase, both claddings show no temperature > 1300 °C.
- The original scenarios lead to significantly higher temperatures with a maximum of app.
 1500 °C (Cr) and 1750 °C (Zirlo).
- Esc. scenario: For the coated claddings the temperature increases significantly above 1300 °C due to the oxidation of pure metal. The optimised Zirlo claddings Temp. rises, forcing a strong oxidation of Zr. When oxidation slows down also the temperatures of both claddings do not escalate strongly.



Simulation Results – Hydrogen Generation



NUBIKI scenario

- Total 4.0 g
- Cr + Zr 0.0 g
- Zr 4.0 g
- Original scenario
 - Total 9.3 g
 - Cr + Zr 3.8 g
- Zr 5.5 g
- Escalation scenario
 - Total 15.0 g
 - Cr + Zr 7.0 g
 - Zr 8.0 g



QUENCH-15

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Test Bundle and Conduct







Simulation Results – Cladding Temperatures at 950 mm



- All simulations reach the transition temperature to accelerated Zr oxidation
- The predicted temperatures for Cr-coating are comparable to original QUENCH-15 Zirlo behaviour



Simulation Results – Hydrogen Generation



- Although the temperature evolution is comparable to QUENCH-15 with Zirlo claddings the mass of hydrogen is less than in QUENCH-15
- During pre-oxidation the hydrogen generation is significantly lower with Cr-coated components
- The increase of hydrogen is strongly connected to the transition temperature in each simulation
- When Zr oxidation occurs after failure of Cr-coating the hydrogen generation is higher than for Zirlo claddings with pre-oxidation



Conclusions

- Currently investigated ATF concepts like FeCrAI and Cr-coating are topic of several international projects and activities. Well known scenarios are applied for bundle configurations with FeCrAI or Cr-coated rods.
- AC²/ATHLET-CD and ASTEC were enhanced for FeCrAI and Cr-coated claddings.
- The application of both codes on different bundle experiments dealing with FeCrAI and Cr-coatings show that both codes can predict the observed test behaviour regarding temperature evolution and hydrogen generation. The results obtained for QUENCH-19 with FeCrAI claddings show a significant improvement of the model basis in the last two years.
- The predictions for CODEX-ATF1 with AC²/ATHLET-CD show a significant impact of the Cr-coatings when the coating fails and pure metal can oxidise.
- Both codes were also applied on a QUENCH test, assuming a Cr-coating. The simulations show that compared to the reference scenario with optimised Zirlo the hydrogen generation is lower in total, but higher above 1300 °C when Cr coating fails. In that phase the temperatures rise but do not escalate as expected in the predictions.
- In general, the validation basis for ATF namely FeCrAI and Cr-coating is limited for bundle experiments and needs an enlargement to evaluate the model basis for ATF claddings in severe accident codes and to further improve the phenomenological understanding, also with respect to eutectics.



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