

# Light Water Reactor Sustainability Program

## Safety Analysis of Chromium-Coated Accident-Tolerant Fuels with Increased Enrichment and Extended Burnup for PWRs



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# **Safety Analysis of Chromium-Coated Accident-Tolerant Fuels with Increased Enrichment and Extended Burnup for PWRs**

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## EXECUTIVE SUMMARY

The U.S. nuclear industry is facing a strong challenge to maintain regulatory-required levels of safety while ensuring economic competitiveness to stay in business. Safety remains a key parameter for all aspects related to the operation of light-water reactor nuclear power plants (NPPs), and it can be achieved more economically by using a risk-informed ecosystem, such as that being developed by the Risk-Informed Systems Analysis Pathway under the U.S. Department of Energy Light Water Reactor Sustainability Program. This program is promoting a wide range of research and development activities to maximize both the safety and economically efficient performance of NPPs through improved scientific understanding, especially given that many plants are considering a second license renewal.

The Risk-Informed Systems Analysis Pathway has two main goals:

- Deploying methodologies and technologies that enable a better representation of the safety margins and factors that contribute to cost and safety
- Developing advanced applications that enable cost-effective plant operation.

As part of this pathway, the Enhanced Resilient Plant project refers to an NPP where safety is improved by implementing various measures, such as accident-tolerant fuels, diverse and flexible coping strategies, enhancements to plant components and systems, incorporation of augmented or new passive cooling systems, and utilization of advanced battery technologies. The objective of the Enhanced Resilient Plant project is to use novel methods and computational tools to enhance existing reactors' safety while reducing operational costs.

This report documents research and development conducted in support of deploying accident-tolerant fuels. Specifically, the performance of chromium coating during a beyond design basis accident was investigated. An 18-month reference core was considered, and the performance of cases with and without chromium coating was compared. An extended cycle length of 24-month was then considered with the chromium coating to determine whether the benefit of using the chromium coating was more or less significant than the increased fission product inventory when considering fission product release. The chromium coating model utilized here is a preliminary implementation, and further work is recommended on a more detailed model.

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## ACRONYMS

ATF	accident-tolerant fuels
BDBA	beyond design-basis accident
ERP	Enhanced Resilient Plant
FFRD	fuel fragmentation, relocation, and dispersal
FP	fission product
FY	fiscal year
HBU	high burnup
HPSI	high-pressure safety injection
INL	Idaho National Laboratory
LBLOCA	large-break loss-of-coolant accident
LOCA	loss-of-coolant accident
LPSI	low-pressure safety injection
LWR	light-water reactor
MACCS	MELCOR Accident Consequence Code System
NPP	nuclear power plant
NRC	U.S. Nuclear Regulatory Commission
PRZ	Pressurizer
PWR	pressurized-water reactor
RAVEN	risk analysis virtual environment
SBLOCA	small-break loss of coolant accident
SOARCA	state-of-the-art reactor consequence analyses
SCALE	standardized computer analyses for licensing evaluation
TEDE	total effective dose equivalent
UDM	user defined material
VERA-CS	virtual environment for reactor applications
WBN	Watts Bar nuclear power plant



# 1. INTRODUCTION

The U.S. Department of Energy’s Light Water Reactor Sustainability Program, Risk-Informed Systems Analysis Pathway, Enhanced Resilient Plant (ERP) project aims to enhance both the safety and economics of existing nuclear power plants (NPPs) using advanced, near-term technologies that provide substantial improvements to plant safety margins. The project supports the Department of Energy and industry initiatives targeting improvements in the safety and economic performance of the current fleet of NPPs, such as accident-tolerant fuels (ATFs), diverse and flexible coping strategies, passive cooling system designs, and advanced battery technologies. The ERP concept refers to an NPP where safety is improved by implementing various measures, such as those described in the previous sentence. The objective of the ERP research is to use novel methods and computational tools to enhance existing reactors’ safety while reducing operational costs. From fiscal year (FY) 2023, the project is focusing on the safety assessments of ATFs with increased enrichment and extended burnup (i.e., high burnup [HBU]), which is an urgent near-term industry initiative that offers safety enhancements as well as economic gains [1]. This work could serve as a roadmap for safety analyses that NPPs must include in their license amendment requests supporting the use of ATFs. Previous reports in FY 2023 have considered FeCrAl cladding in pressurized-water reactors (PWRs) with UOX fuel. In FY 2024, this work was extended to consider chromium-coated zircaloy cladding.

The possibility of higher burnup is more achievable with ATF compared to the traditional Zr clad fuel due to ATF’s more robust cladding properties to cope with accident conditions. In this context, extended HBU operation up to 24 months can provide a significant economic benefit for operating nuclear reactors. However, ATF development is still ongoing along with the enhancement of the modeling and simulation capabilities that can provide sufficient information about how HBU ATF performs under accident scenarios. The safety analyses of HBU ATF are still incomplete, especially in terms of fuel performance. The fuel cladding failure could occur during postulated accident events and may cause fuel damage exceeding the regulation safety limits. The main limiting degradation phenomena are the cladding deformation and fuel fragmentation, relocation, and dispersal (FFRD). Cladding deformation is possible during a loss-of-coolant accident (LOCA).

FY-2024 research focused on the safety analysis of ATF, specifically chromium-coated zircaloy cladding, with increased enrichment for the higher burnup fuel-cycle operation. A beyond design-basis accident (BDBA) (e.g., severe accident) is considered—addressed in NUREG-0800, “Standard Review Plan for the Review of Safety Analysis Reports for Nuclear Power Plants: LWR Edition” [2]. In FY 2023 [3], the project also performed a consequence analysis from released radioactivity across the engineered safety boundary and to the environment for the FeCrAl case. The consequence analyses support understanding changes between the conventional Zr clad fuels as related to NUREG-1465 [4], which was developed for the conventional Zr clad fuel with lower burnup, and ATF-clad fuels. While the consequence analysis was not performed here, the methodology is readily extendable to this. This work could serve as a roadmap or reference for safety and consequence analyses that NPPs must include in their license amendment requests for an HBU fuel-cycle operation.

## 2. ANALYSIS ON THE BEYOND DESIGN-BASIS ACCIDENT

In this section, a brief description of the BDBA model is provided. This was also provided in the FY-2023 report [3] but is reproduced here for convenience. An analysis was performed for a severe accident analysis that was initiated from a recovered large-break loss-of-coolant accident (LBLOCA) focusing on the source term by using MELCOR [1]. This recovered LBLOCA scenario intentionally delays the LPSI activation time to damage core for source term analysis which was used as standard test problem of U.S. Nuclear Regulatory Commission (NRC) (e.g., SOARCA report) [5].

The analysis includes both 18- and 24-month fuel cycles for Zr clad fuel with and without Cr-coating. The fission product inventory was calculated from the SCALE core lattice modeling code and VERA-CS high-fidelity depletion calculation tool [1]. The fission product inventory and decay heat data were developed for a 24-month cycle.

The source term consequence analysis has more meaning in a relative sense. In the previous study, the amount of major source terms was less in an accident in a PWR with FeCrAl-clad fuel compared to Zr clad fuel during both the 18- and 24-month cycles [1]. From this result, it is expected that the environmental impact will be lower when using ATF clad. However, this low environmental impact of ATF is not an authoritative indication of the source term decrease; instead, the fission product inventory is much higher in the higher burnup fuel cycle. The relative impact of an increased burnup and cladding material change will be different in other severe accident scenarios. During a severe accident initiated by a LBLOCA, the accident consequences may be very similar between lower and higher burnup cases, but higher burnup fuel will produce a larger fission product inventory. However, the released source term amount from ATF was found to be lower than Zr clad fuel since ATF shows smaller damage rate compared to Zr clad fuel [1].

### 2.1 Model Description

#### 2.1.1 Reactor Design

Figure 1 shows a diagram of the Westinghouse four-loop PWR Watts Bar NPP (WBN-1) Cycle 1 full-core layout on the left with an axial layout (which is publicly available data) of the fuel assembly on the right, which has similar power configuration with Zion NPP and used as the base of the reactor core design in MELCOR [1]. This core is filled with 193 fuel assemblies and has a rated thermal power of 3,411 MW. The main operating parameters of this core are shown in Table 1.

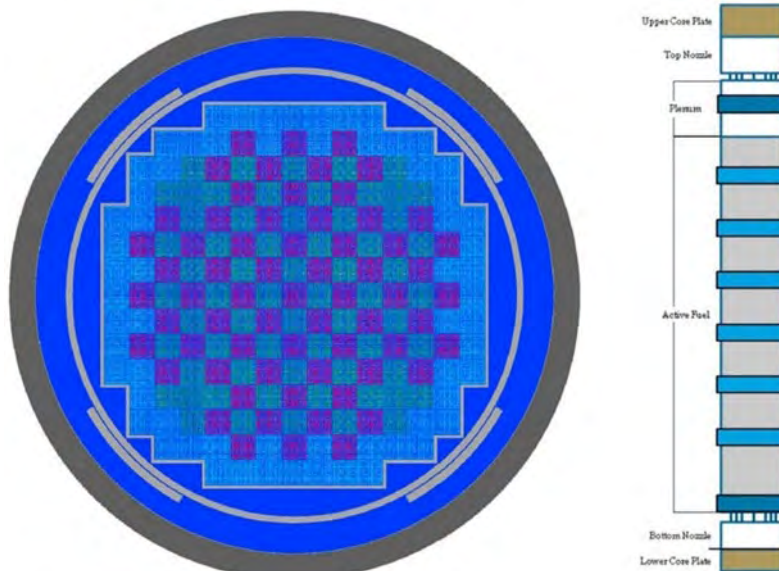


Figure 1. WBN-1 core diagram.

Table 1. Core characteristics for the generic PWR.

Parameter	Value
Rated thermal power (MWth)	3,411
Rated flow (kg/s)	18,231
Inlet temperature (K)	565
Coolant average temperature (K)	585
System pressure (MPa)	15.51
Coolant core bypass flow rate (%)	9.0

The fuel assembly used in this analysis consists of a conventional  $17 \times 17$  lattice of fuel rods. In previous work [1], an equilibrium core was derived using VERA for an 18-month core with zircaloy clad and a 24-month core with FeCrAl clad. The core power distribution is used as an input to MELCOR. The enrichment and end-of-equilibrium cycle discharge burnup are used as inputs to a single assembly SCALE calculation that is used to derive the end-of-cycle inventory. With Cr cladding, the penalty to enrichment is small (of the order of 0.1%) [6]. The same inventory and discharge burnup is, therefore, used for the Cr-coated case as for the reference Zr case. For the 24-month case, in principle, it is more accurate to derive a 24-month core containing Zr cladding (potentially with Cr-coating). This was not available for the present work, so instead we use the FeCrAl cladding 24-month core power distribution. The SCALE calculation is performed with an enrichment of 6.3% for the 24-month core. This is calculated by taking the difference in enrichment between the FeCrAl and Zr 18-month cores (i.e., the enrichment penalty from using FeCrAl) and subtracting it from the enrichment for the FeCrAl 24-month core, adjusting for the slight Cr-coating penalty. While approximate, this approach is reasonable as the decay heat and fission product inventory are dominated by the core power burnup (which is a function of core power and cycle length).

## 2.1.2 Modeling Beyond Design-Basis Accident Scenarios

The WBN-1 reactor core model was applied to the MELCOR Zion NPP model as defined in the original NRC's severe accident analysis model [5]. The model was revised for the source term analysis which includes recovered LBLOCA scenario. Input detail is not publicly available. The systems model of the reactor is shown in Figure 2. MELCOR constructs a list of control volumes containing important systems, defines flow paths between these volumes, and specifies materials and interactions occurring in the plant. In addition, the radial and axial nodalization schemes of the core are shown in Figure 3, which is built using the COR package in MELCOR. Note in the "Results and Discussion" section, the active cells will be labeled as "Cell-1" to "Cell-11," which starts for each ring from "L8" to "L18" as described in Figure 3.

The accident time sequential is given in Table 2. The accident scenario assumed that the emergency core cooling system initially failed and the LPSI system was reactivated at 27 minutes (1,620 seconds). The simulation will end at T + 6 hours (21,600 seconds). The accident time sequential was the same for both the 18- and 24-month cycle and Zr- and FeCrAl-clad fuel models.

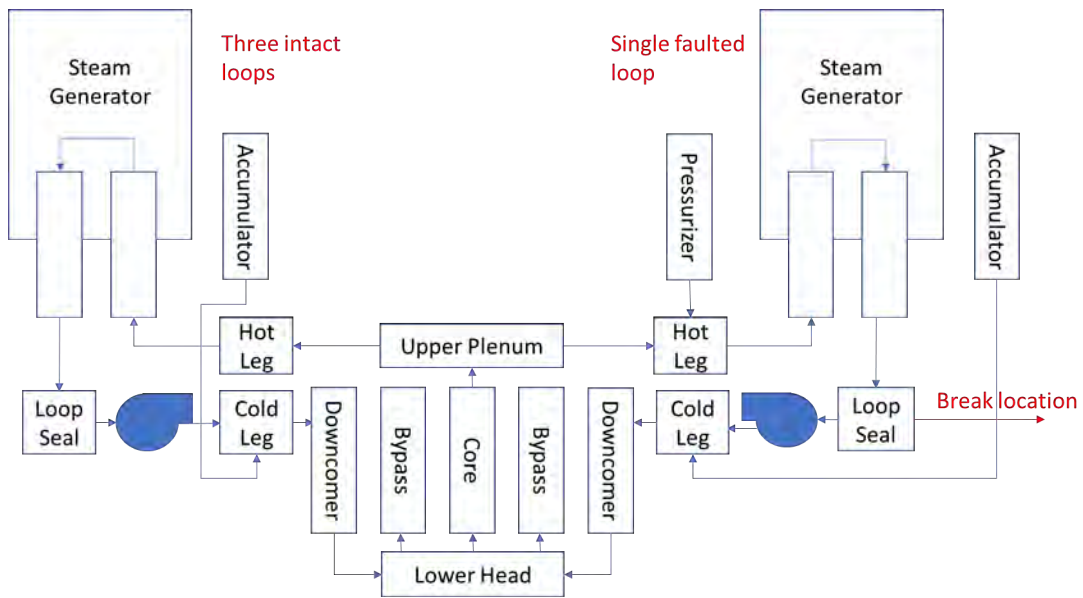


Figure 2. Nodalization for MELCOR modeling.

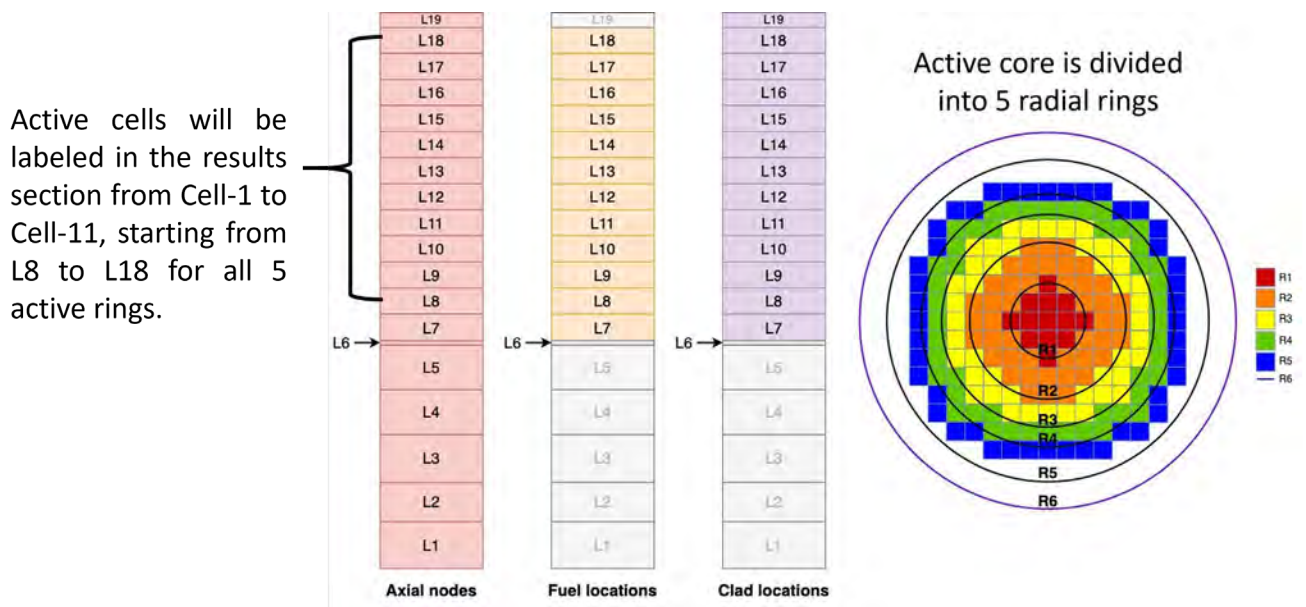


Figure 3. Axial and radial nodalization scheme used in MELCOR.

Table 2. Time sequential of the MELCOR LBLOCA scenario.

Event	Time (s)
Simulation starts	T - 200
Double-ended rupture in PRZ loop	T + 0
Reactor SCRAM	T + 0
Accumulator activation	T + 40 (at 4.275 MPa)
LPSI reactivation	T + 1,620
LPSI ends	T + 2,004
Simulation end	T + 21,600

### 2.1.3 Oxidation Model for Cr-Coating Zr-Based Cladding

In the past, MELCOR required a special cladding/oxidation model to be implemented in MELCOR to capture the advantage of the ATF cladding that replaced Zr. B.J. Merrill et al. [7] modified a version of MELCOR to allow a material other than Zr to be the outermost material in the clad until it fails/oxidize then MELCOR shifts back to the Zr characteristics. Hence, it was possible to compose the cladding out of two materials to model coated/wrapped cladding.

Currently, the MELCOR version 2.2.21402 (a release of the mainline version developed by Sandia National Laboratories) used in this study has not adopted the above-mentioned modification. Therefore, a different approach is considered in this work by creating a homogeneous-material (HM-model) as a cladding material (Zr+Cr). This is performed by defining the percentage of each material's mass, based on the initial thicknesses and assumed Zr thermo-physical properties. This homogeneous material is defined as a cladding material in MELCOR using the user-defined-material function. Moreover, the oxidation model in the presented approach is composed of two different sets of oxidation parameters for Zr and Cr, which is significant for simulating the oxidation process. That was not possible when only the temperature dependency is considered as addressed by Wang et al. [8]. That is because MELCOR does not provide access to these parameters using the control-function package; whereas, the HM-model provides the opportunity of having two distinct set of oxidation parameters as listed in Table 3. In addition, each oxidation model activates based on the temperature range (Table 4). Hence, for temperatures range between 1100 – 1603 K, the Cr oxidation model is activated; while greater than 1603 K, the Zr oxidation model is activated, simulating the temperature beyond which the Cr-coating can be assumed to stop being effective. The 1603 K is specified based on the eutectic temperature of Cr-Zr as reported in [9]. Moreover, this modeling approach permits MELCOR to alternate between the two oxidation processes locally (cell by cell), without overriding the oxidation kinetics of all the other cells. The logic of the adapted cladding model in this work is presented in Figure 4.

Table 3. Oxidation parameters for Zr and Cr [10], [11].

Metal Material	Parameter	Value
Zr	Chemical Equation	$Zr+2H_2O>ZrO_2+2H_2$
	Heat of Reaction	5.797E+06 J
	Diffusion Constant	0.00548 kg/(mol.J)
Cr	Chemical Equation	$Cr+1.5H_2O>0.5Cr_2O_3+1.5H_2$
	Heat of Reaction	2.666E+06 J
	Diffusion Constant	0.00161 kg/(mol.J)

Table 4. Oxidation kinetics with respect to temperatures ( $K(T) = \alpha \cdot e^{-\frac{\beta}{T}}$ ) [10], [11].

Metal Material	Temperature Range (K)	$\alpha$ (kg/m <sup>2</sup> /s)	$\beta$ (K)
Zr	1100-1323	0.0	0.0
	1323-1603	276.84	41374.4
	1603-9900	0.0	0.0
Cr	1100-1603	0.0	0.0
	1603-1853	29.6	16820
	1853-9900	87.9	16610

It is worth noting that in all the presented investigation, the standard eutectic model that is specific for the Zr cladding is disabled. This is because the Zr eutectic model is not compatible with the UDM approach, and therefore, it should be disabled for consistency between Zr and ATF cladding models. This treatment was also used in the previous phase of work where Zr and FeCrAl were compared [1]. It is worth emphasizing that there is insufficient knowledge when it comes to understanding the metallic interaction of the Cr and Zr. This requires further experimental research to help implementing a Zr-Cr eutectic model in MELCOR and similar codes.

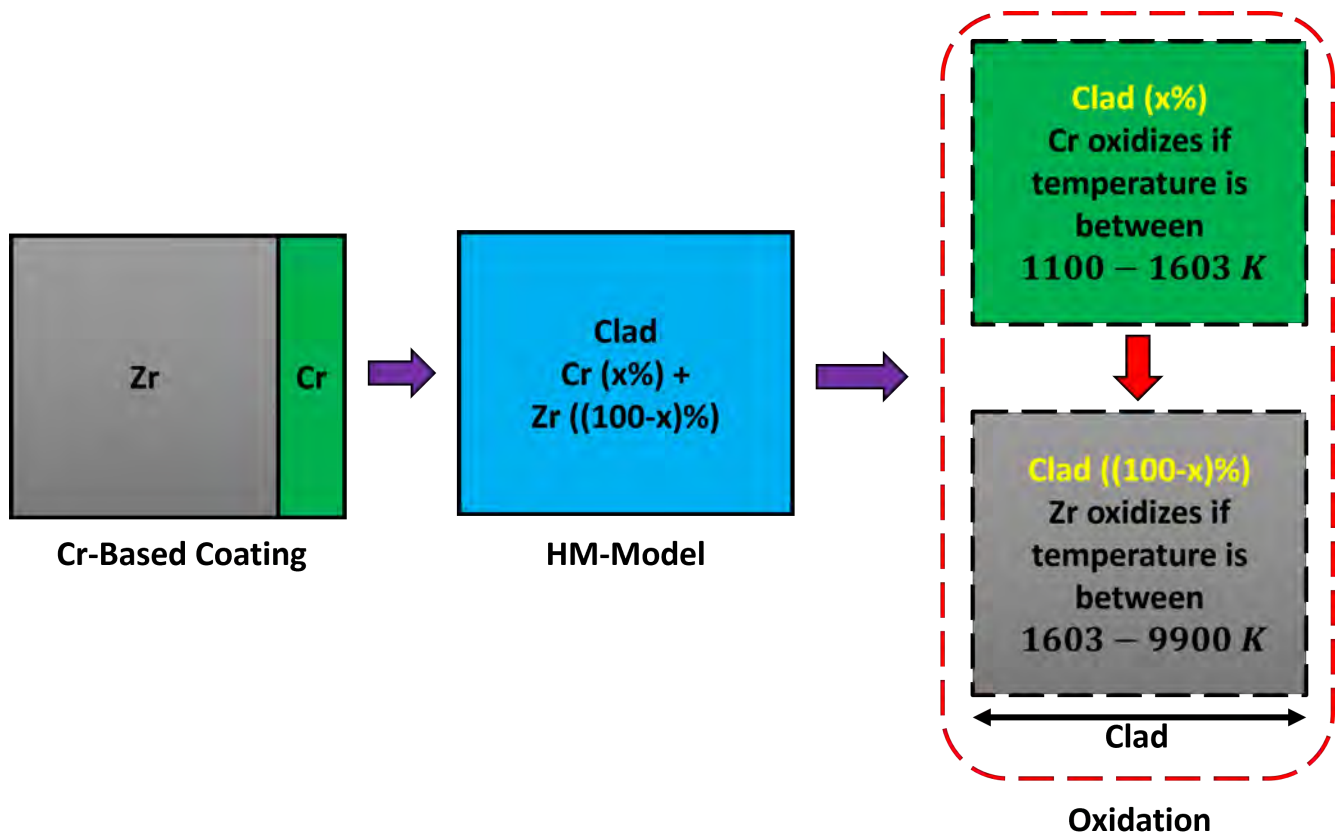


Figure 4. Scheme showing how the Cr-based Zr cladding is modeled.

## 2.2 Results and Discussion

The significance of the Cr-coating is investigated by developing eight ZION models in which they differ in the cladding (Zr-based, Cr-coating: 6, 18, and  $28\mu m$ ) and the fuel cycle (18 and 24-months). To explore the significance of the Cr-coating, first, a comparison between the 18-months Zr-based model and the Cr-coating-Zr ( $18\mu m$ ) model is conducted on a local (COR-cell) basis. Before discussing the temperature profiles presented in Figure 5, it is worth noting that the Zr cladding failure temperature of the clad is specified in MELCOR as 2500 K (the default value) which is the failure based on the temperature and remaining thickness of the structural metal. Besides, since the Cr-coating amount makes only 1% to 5% of the total clad, the failure temperature is assumed to remain the same for both the Zr-based and the Cr-coating Zr claddings. Figure 5-A shows how the temperature evolution is very similar in ring 1 for the two models with a slight delay in time for a certain cell to reach the failure temperature ( $\sim 1$  min). In this transient, this indicates that the Cr-coating impact does not prevent significant melting due to the fast rate of heating that ring-1 has been exposed to.

On the other hand, in the other rings, where the transient is occurring at a slower rate, the impact is more pronounced as can be seen in Figures 5-B and 5-C. For example, in Figure 5-B, although the melting has occurred partially in ring-3, the heating of the cladding is more significant in the case of the Zr-based cladding compared to the Cr-coating-Zr cladding model for cells 1 to 5. Hence, it takes remarkably less time for cells 1 to 5 to cool down after the water reinjection. This can be attributed to the significant difference in the heating rate influenced by the oxidation behavior. One can observe it from the behavior of the  $H_2$  generated due to oxidation in these cells, as shown in Figure 6-A. In addition, Figure 6-B shows how there is a slight generation of the  $H_2$  in case of Zr-based model in ring 5, leading to a clad temperature increase  $> 100 K$  (Figure 5-C) compared to the Cr-coating-Zr cladding model. In the Cr-coating-Zr cladding, the temperature remains below 1323 K, and therefore, there is no  $H_2$  generation implying that no oxidation phenomenon took place.

Furthermore, the difference in the oxidation behavior has led to a difference in how the cladding relocates after failure (melting). As can be seen in Figure 7, the cladding mass relocates and accumulates in cells 1 and 2, while in the case of the Cr-coating-Zr cladding model, the cladding mass accumulates in cell 5. This can be due to the shorter time for the cells to cool down resulting in a faster solidification of the clad, before reaching the bottom cells. As discussed previously, this is a result of the excessive oxidation heat released in the case of Zr-based cladding model.

The results of the liquid level in each control volume in which the different active cells are located (Figure 8) show that there is a faster development of liquid in the upper region (cells 9-11) after reinjection and a much slower rate in the lower control volumes. This phenomenon will be explored further in future research, as it is not clear yet what may have led to it. The current hypothesis relates this to a possible counter flow in the reactor core, which can be described as follows: as the hot molten mass is accumulated in the lower regions, and the water is reinjected (from the top), the water easily goes through the upper region but instantly evaporates as it enters the lower regions due to the high temperatures of the accumulated mass. Besides, by comparing the two models, the Zr-based cladding model manifests a higher liquid level in the control volume of cells 3–5 compared to the Cr-coating-Zr cladding model. This can be explained from relocation of the cladding mass presented in Figure 7, large amount of cladding mass is accumulated in cell 5 for the Cr-coating-Zr cladding model, unlike the Zr-based cladding model, where the accumulation is in cells 1 and 2. This observation can support the introduced explanation. However, the current results are not sufficient to validate this hypothesis, and more research investigating the thermal-hydraulics behaviors is required (for example, investigating the flow paths in various channels in the model).



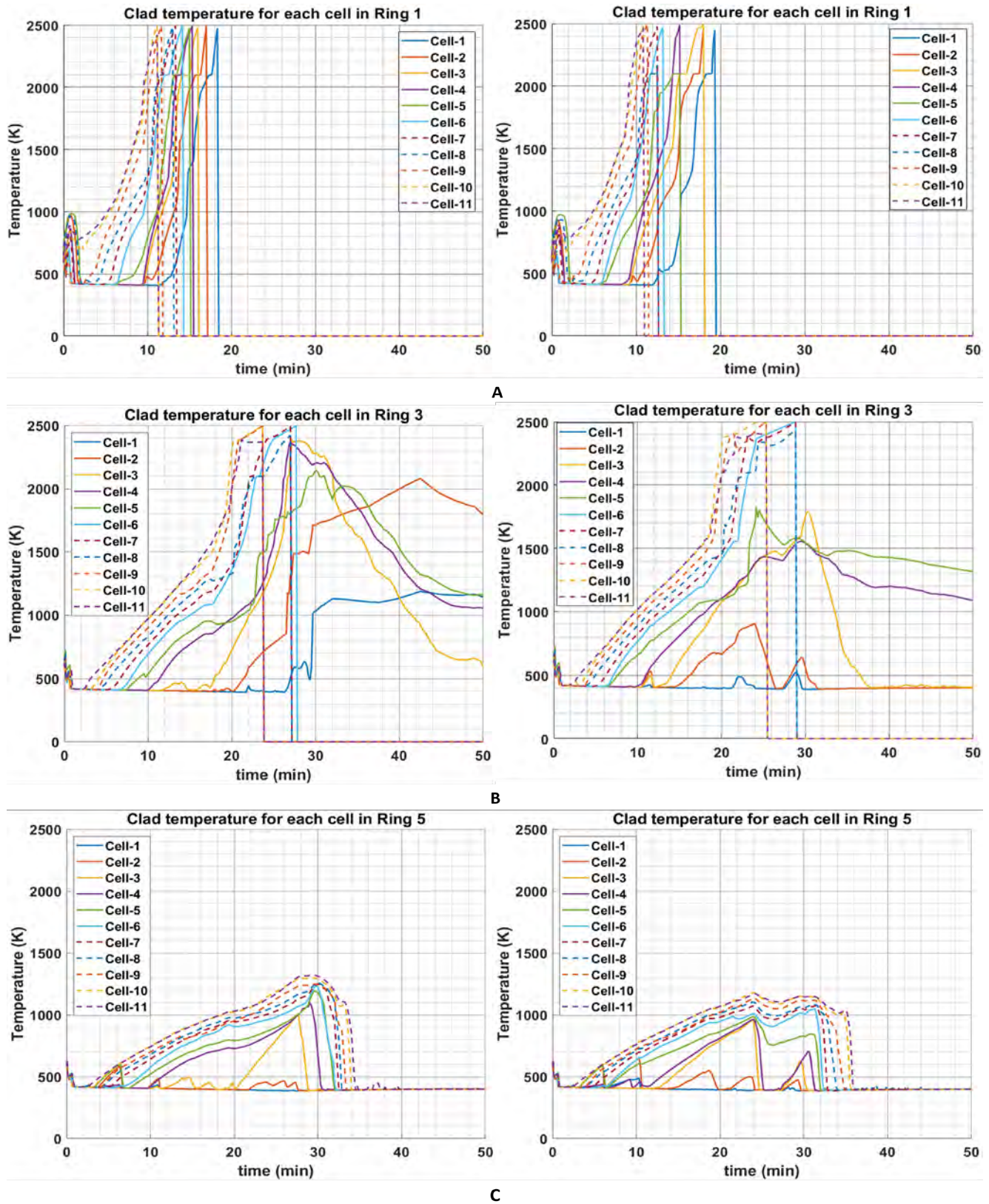


Figure 5. Temperature changes over time for different cells. Left-figure: Zr-based cladding model, 18-months. Right-figure: Cr-coating-Zr (18 μm) cladding model, 18-months.

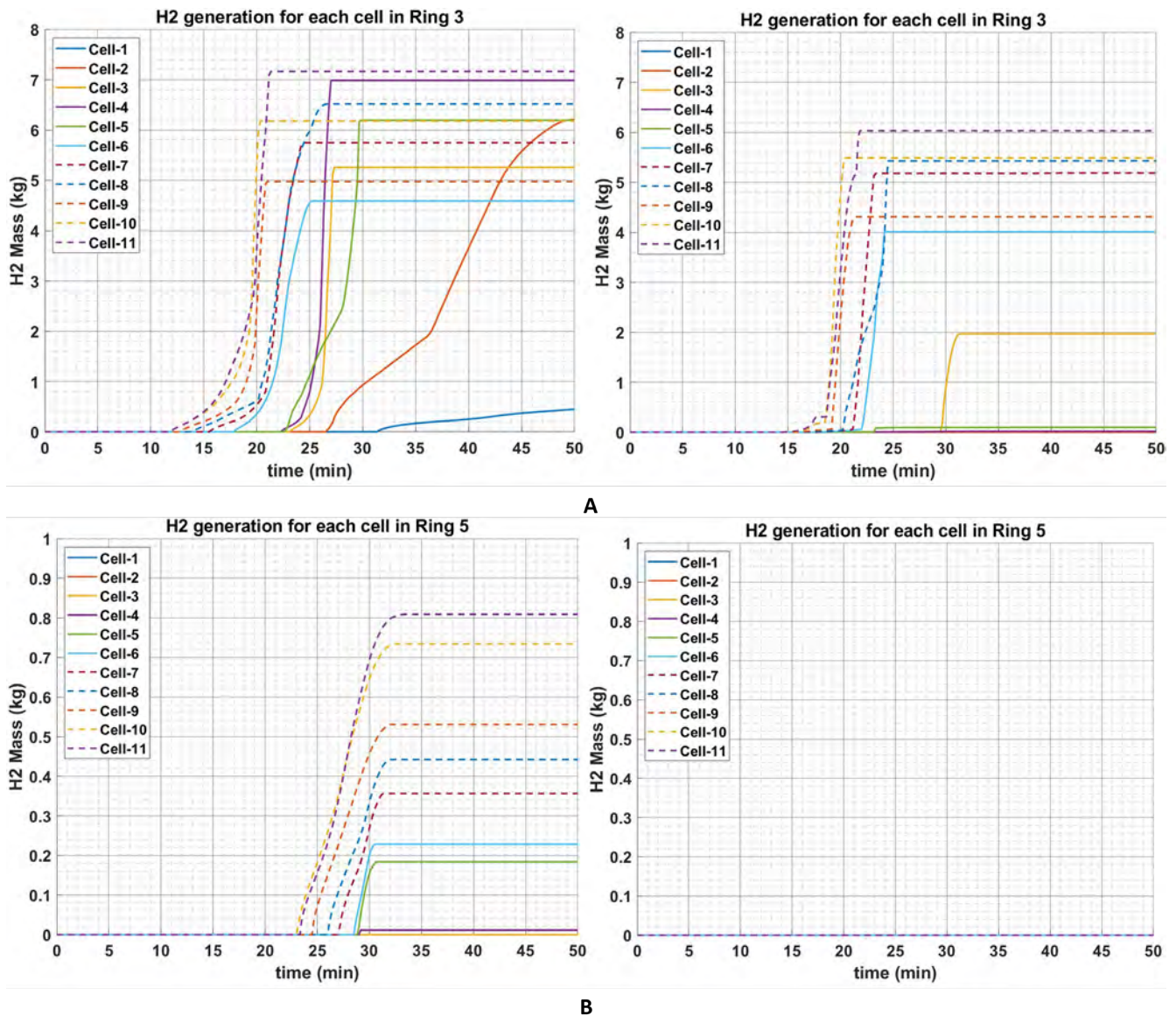


Figure 6. H<sub>2</sub>-generation due to oxidation over time for different cells. Left-figure: Zr-based cladding model, 18-months. Right-figure: Cr-coating-Zr (18  $\mu\text{m}$ ) cladding model, 18-months.

The significance of Cr-coating for different axial and radial segments in the core is more pronounced by examining the global impact on the core's transient behavior. The results show that even with the 24-month fuel cycle, the total fission products (FPs) released is still beneath the total FPs released with the 18-month Zr-based cladding model (Figure 9-A). Furthermore, there is a significant reduction in the total generation of H<sub>2</sub> (Figure 9-B), leading to a reduction in the heat released from the oxidation (Figure 9-C). This results in a reduction of the overall core damage, as shown in Figure 9-D. Hence, the Cr-coating has the potential to facilitate extending the fuel-cycle length through recapturing extra margin.

In addition, it can be understood from Figure 9 that the Cr-coating thickness may cause remarkable impact in the outcome, even for small thicknesses. Interestingly, the Cr-coating of 6  $\mu\text{m}$  has caused the most impact on reducing the total FPs release and damage in case of the 18-month fuel cycle. However, the Cr-coating was found to have the most impact for the 24-month fuel-cycle case. The results may suggest that the impact of the Cr-coating thickness depends on the power distribution, fuel cycle, FPs inventory, etc. However, it must be noted that



the current model has limitation in capturing the effect of different thicknesses. Specifically, the current model treats any given volume of the cladding that is exposed to the steam as  $x\%$  of Cr and  $(100-x)\%$  of Zr; whereas in practice, Cr would be occupying 100% of the volume up to a certain thickness (the coating thickness). This leads to an underestimation of the amount of oxidized Cr, which results in underestimating the heat produced, which eventually results in an overestimate in overall core damage. This overestimation in core damage is less significant with larger amount of Cr considered, which is reflected in Figures 9-B and 9-C. Therefore, further works should consider the inclusion of a mass transfer criterion, in addition to the temperature criterion of the HM-model developed here. Unfortunately, it is not possible to consider that with the current MELCOR version; hence, a recommendation to MELCOR's development is made in Section 3.

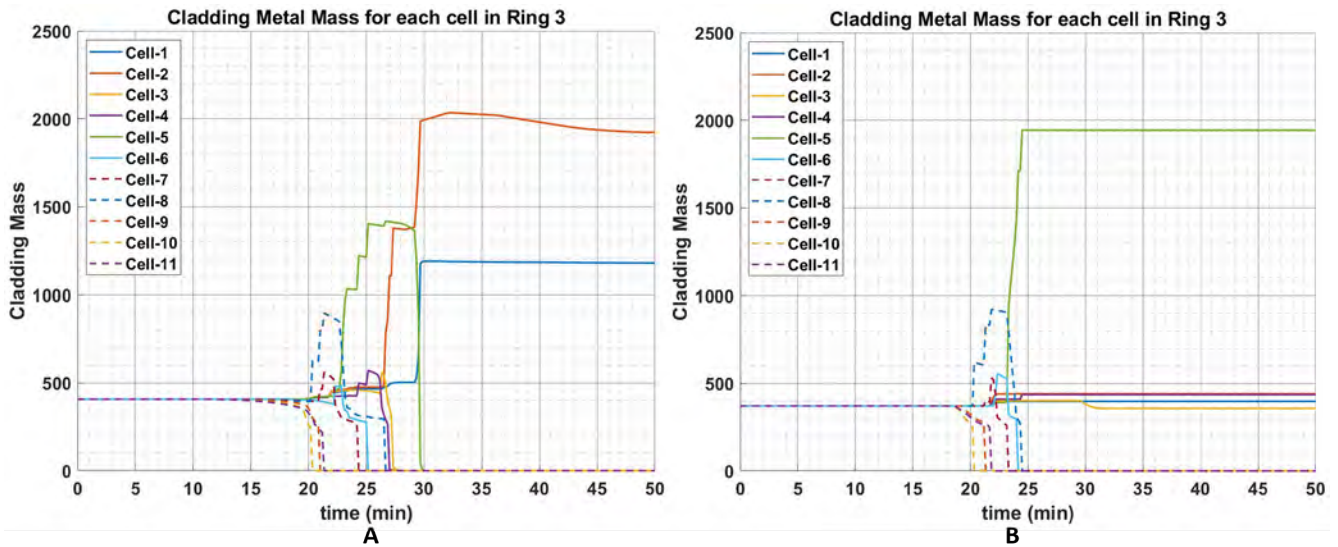


Figure 7. Behavior of the cladding mass relocation over time for different cells. Left-figure: Zr-based cladding model, 18-months. Right-figure: Cr-coating-Zr ( $18 \mu m$ ) cladding model, 18-months.

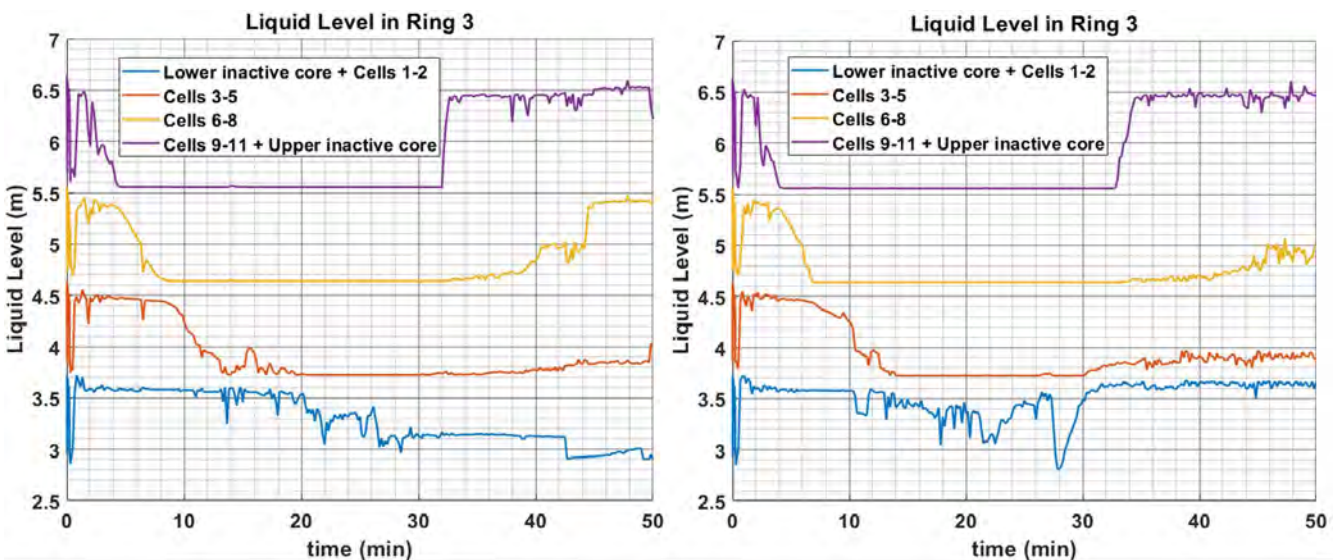


Figure 8. Behavior of the liquid level over time in different control-volume levels. Left-figure: Zr-based cladding model, 18-months. Right-figure: Cr-coating-Zr ( $18 \mu m$ ) cladding model, 18-months.

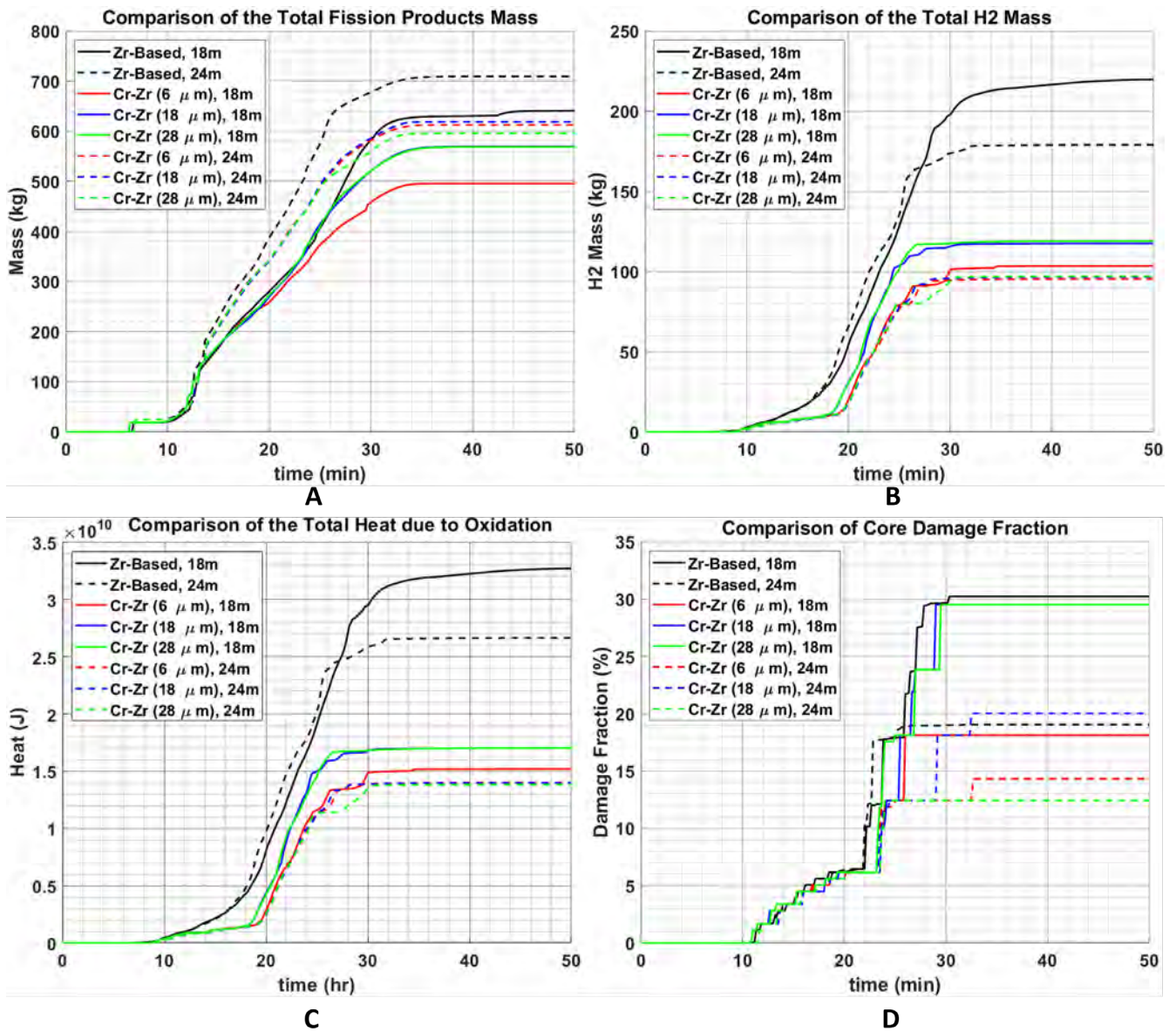


Figure 9. The difference in the global behavior corresponding to different models that differ in the cladding and fuel cycle.

### 3. CONCLUSIONS AND FUTURE WORK

The analysis of Cr-coated Zr for beyond design-basis transients has been demonstrated in principle here with the state-of-the-art version of MELCOR 2.2.21402. A homogeneous model for Cr-coated Zr has been developed within MELCOR, which benefits from the user-defined-material feature in MELCOR. In this model, the kinetics of the oxidation depend on the temperature of the cladding; however, the oxidation process is composed of two distinct oxidation processes depending on the material. Implementing two different oxidation models found from the presented results to be crucial in capturing the role of Cr significance, particularly in evaluating the heat released and H<sub>2</sub> production. However, the developed model has some limitations associated with this method, due to the lack of mass-dependency, and inability to be flexible in capturing the effect of different rates of cladding heating.

That being said, the model has been useful in simulating the impact of the Cr-coating oxidation in a physical sense, especially in case of slow heating rates. The results show there is a significant reduction in the oxidation, leading to a reduction in the heat released, which results in the reduction of the overall core damage, and a shorter time required to bring down the temperatures of the cladding in case reinjection is performed after severe accident. Additionally, the total FPs released in a 24-month Cr-coating core is still beneath the total FPs released with the 18-month Zr-based cladding. Hence, the Cr-coating has the potential to facilitate extending the fuel-cycle length through recapturing extra margin.

With respect to the source term analysis work performed here, the following future works (short-term) are recommended to enable a more correct representation of the dynamics of coated cladding oxidation:

- The Cr-coating model utilized here is based on temperature dependence. This is a reasonable approximation for the purpose of this work but does not capture differences in behavior during slow and fast transients based on how long it takes for the Cr layer to oxidize and eventually fail. In principle, a model based on oxidizing the Cr first and then the Zr is possible in MELCOR, and this approach may be more accurate. It is recommended that this feature be completed in MELCOR and then utilized for the model presented here and compared to the temperature dependence approach.
- A more sophisticated treatment is possible by having a “**multi-layer**” **cladding material**, established in the latest versions of MELCOR, where the order of oxidation can be specified to avoid having oxidation that occurs simultaneously for both materials (Cr-Zr).
- To demonstrate an overall reduction (or lack of increase) in a source term with respect to the reference case, the next step is to **propagate the fission product release to an accident consequence analysis**. In the United States, 10CFR50.67 states that when evaluating “proposed design basis changes with respect to potential reactor accidents of exceedingly low probability of occurrence and low risk of public exposure to radiation,” a reference value of 0.25 Sv total effective dose equivalent (TEDE) may be used for an “individual located at any point on the boundary of the exclusion area [10 miles] for any 2-hour period following the onset of the postulated fission product release” [12]. This comparison was performed in FY 2023 for FeCrAl fuel, using the MACCS (MELCOR Accident Consequence Code System) code to propagate results from MELCOR to analyze accident consequences [1]. This could also be performed for the Cr-coating, which probably most useful to show that Zr source terms are bounding relative to Cr-coated cladding source terms at higher burnup, and possibly under uprated conditions.
- A wider range of transients could be analyzed, and sensitivity and uncertainty analysis could be performed. This could include (for example) a station blackout (SBO). Also, the sensitivity of results to transient progression could be investigated, including sensitivity to the LPSI reactivation time. Ultimately, the consequences for multiple transients could be evaluated and weighted by their respective probabilities to calculate an overall source term. Then, the source term can be compared between Cr-coated HBU fuel and Zr fuel. Furthermore, in our previous work, RAVEN was used to

perform uncertainty analysis for FeCrAl clad. A similar methodology could be applied for the Cr coating investigation. Besides, DAKOTA is an alternative tool that could be utilized as well.

The following future works (long-term) are recommended to produce more data that can help in a better understanding of the ATF concepts impact:

- The results of this work emphasize the importance of conducting an experimental investigation that explores the significance of the Cr-coating role under different transient conditions, particularly exposure to slow-to-fast heating, in addition to the consideration of early, late, or no-reinjection. This is essential in widening our scope where the Cr-coating cladding is more advantageous and when it is not. Moreover, because, the current understanding is that the oxidation process is a function of temperature, therefore, **obtaining such experimental data** can help in developing a more robust Cr-coating model, which would include the temperature temporal effect, to have a model that can capture different transient behaviors.
- **Intermetallic interactions between dissimilar core materials** have indicated the potential for onset of melting at temperatures lower than the pure material melting points of interacting core materials. With the introduction of new materials into the reactor core, the potential for occurrence of earlier melting of core structures must be considered to obtain a more realistic representation of degradation and associated fission product release from fuel. Are there, for example, intermetallic interactions between Cr and underlying Zr that lead to early melting of the cladding? What is the degree of melting should intermetallic interactions occur? While experimental efforts are essential, initial progress in this area could be made through evaluations of the equilibrium thermochemical phase diagram corresponding to the interacting materials.

More generally, ATF concepts have received attention primarily related to performance under the early phases of an accident where traditional fuel cladding would begin to experience oxidation. The state-of-knowledge on the behavior of ATF concepts beyond this early phase of an accident, into more severe conditions leading to fuel degradation, is more limited. While there are experimental programs currently acquiring some relevant data (e.g., the OECD/NEA QUENCH-ATF program [13]), the current understanding remains limited by the sparsity of data relevant to phases of the accident at onset or with progressive fuel degradation. The following initiatives represent areas for knowledge advancement to enhance the modeling realism for source term analysis with Cr-coated fuel.

- Currently, there is limited data available to provide insights into how onset of **fuel degradation may differ for ATF concepts relative to the currently deployed LWR fuels**. While cladding oxidation may be delayed across the different ATF concepts, the introduction of new cladding or fuel materials will influence the temperature at which degradation commences. Of particular interest is whether degradation modes emerge at lower temperatures than the existing UO<sub>2</sub>-Zr fuel forms. There is evidence for existing fuel forms that fuel assemblies can experience a structural collapse when exposed to elevated temperatures for a prolonged period. This has resulted in time-at-temperature lifetime models being implemented in severe accident computer codes. The understanding of these types of modes of degradation typically requires experimental insights, though they may be less dominant than other modes of degradation for new fuel forms.
- **Radionuclide interaction with core materials.** The interaction between radionuclides and materials in the reactor core has been influential in understanding the potential volatility of different fission products. With new core materials, the potential for a change in volatility of key consequential fission products must be assessed in more detail. While uncertainties remain in relevant thermochemical databases, there is an opportunity to explore the impact of new materials (e.g., the presence of more Cr to interact with fission products being released from the fuel) on fission product compounds that could form during an accident.
- As noted in the previous areas for further investigation, state-of-knowledge with respect to fuel and core behavior under severe accident conditions is typically lower for ATF concepts. Though there remain significant uncertainties for the UO<sub>2</sub>-Zr fuel forms, the benchmarking of existing models

against available experiments and reactor-scale accidents have generally found the models to be appropriate for evaluating risk. The global conditions most influential to the estimation of consequences (i.e., fission product release from containment) are generally not strongly influenced by the uncertainties that remain at a finer scale. However, the uncertainties that ATF concepts introduce are in some cases unique and an understanding of how they impact accident progression and source term estimation is important. A model-informed assessment and prioritization of severe accident modeling uncertainties for ATF concepts is valuable not only from the perspective of analysis but also to develop experimental programs having the highest impact.

- To truly assess the impact of new ATF concepts on overall risk, it is important to **perform large-scale Level 2 PRA studies to quantitatively characterize the risk profile**. A first-of-a-kind study characterizing the risk profile for BWRs was performed by EPRI as part of the Containment Protection Release Reduction (CPRR) rulemaking. The modeling and simulation methodology applied in the EPRI study proved essential to evaluate how different radionuclide release mitigation measures or strategies affected the overall risk profile of a typical BWR Mark I. A similar approach can be applied to develop a more realistic understanding of the impact of ATF concepts on a nuclear power plant's risk profile. In the case of ATF concepts, however, additional care will be needed with respect to assessing the impact of critical phenomenological uncertainties.

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