Original Article

Numerical simulation of the effects of localized cladding oxidation on LWR fuel rod design limits using a SLICE-DO model of the FALCON code

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A methodology for evaluation of mechanical and thermal effects of localized non-axisymmetric oxidation in zircaloy claddings on LWR fuel reliability is proposed. To this end, the basic capabilities of the FALCON fuel behaviour code are used. Examples of methodology application to adjustment of selected operational limits for modern BWR fuel rods, to capture effects of the excess local oxidation, are presented. Specifically, the limiting rod internal pressure for the onset of cladding lift-off is reduced, depending on initial excess oxidation spot sizes. Also, the power limits for Anticipated Operational Occurrences are adjusted, to preclude fuel melting and cladding failure due to PCMI and PCI-SCC in the affected fuel rods.

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1. Introduction

The predicated thermo-mechanical effects of low-temperature oxidation of the cladding on LWR fuel reliability and safety are largely caused by the impact of an oxide layer on mechanical and thermal properties of the cladding. Degradation of the mechanical state occurs because the oxide layer is brittle and susceptible to cracking at a cladding tension during Pellet-Cladding Mechanical Interaction (PCMI). Thus, the oxidation results in a reduction of the mechanical-load bearing thickness of the cladding. A thermal effect is due to the reduced thermal conductivity of the zirconium oxide, which is an order of magnitude lower than the thermal conductivity of zircaloy [1]. A thick oxide layer can therefore result in cladding overheating leading to further acceleration of oxidation due to a positive thermal feedback effect.

Localized oxidation of the claddings can be amplified during operation in LWRs due to different mechanisms. The cladding outer surface temperature and, consequently, oxidation rate can be elevated during a temporal boiling crisis, which can eventually lead to dry-out of the cladding outer surface [2]. A similar effect may occur due to redundant crud deposition on the cladding surface [3], which can considerably reduce the effective cladding-to-coolant heat transfer coefficient [4]. Besides, discernible local increase in cladding oxide thickness has been occasionally observed at the spacer levels in BWR fuel assemblies, due to so-called ‘shadow’ corrosion [5].

Redundant oxidation of the cladding during operation in LWRs can eventually compromise fuel reliability. Indeed, original fuel operational limits (see Chapter 2) have been obtained by fuel vendors, largely, based on experimental data and code analysis [6,7]. The corresponding calculation has been performed assuming unaffected, normally operated fuel rods. For the affected fuel, verification or adjustment of the original reliability and safety limits [8] would be necessary to capture potential detrimental effects of the local excess oxidation, if any.

Additional features in the above-mentioned effects are to be accounted for by fuel reliability and safety analysis when oxidation is not azimuthally uniform, meaning e.g. localized excess oxide spots on one side of the cladding with the other side being unaffected. This is particularly feasible for fuel rods operated in BWRs, where considerable non-uniformity of neutron-physical, thermo-hydraulic and thermo-mechanical boundary conditions may arise from specific features of fuel assembly designs [9]. Indeed, most of the fuel behaviour codes employ 1.5-D or 2-D numerical solution
methods assuming axisymmetric, azimuthally uniform distribution of the boundary conditions and material properties [10], which may be insufficient for adequate simulation of the features just mentioned.

To cope with simulation of the effects of localized non-axisymmetric oxidation in zircaloy claddings on LWR fuel reliability, special models and a methodology, using basic capabilities of the FALCON code [11], have been developed at Paul Scherrer Institut (PSI – Switzerland), which is described in Chapter 3 of the current paper. Examples of methodology application for adjustment of the selected operational limits of modern BWR fuel rods, to capture the effects of the excess local oxidation of the cladding are presented in Chapter 4.

2. Fuel rod design criteria and operational limits

2.1. Background

In general, the fuel design (safety) criteria [8] are defined by fuel vendors (or safety regulators) with the purpose of avoiding fuel transition into physical states that may compromise its reliability and safety, e.g.: fuel pellet melting, cladding ‘lift-off’ due to high internal gas pressure, redundant cladding corrosion, cladding failure caused by Pellet-Cladding Interaction (PCI) assisted-Stress-Corrosion Cracking (SCC) or Pellet-Cladding Mechanical Interaction (PCMI) during Anticipated Operational Occurrences (AOOs), etc. To this end, and in accordance with the current practice, fuel vendors impose fuel-rod design specific limits on operational conditions to be observed by the operator, i.e. a Nuclear Power Plant (NPP). Most frequently, constraints are imposed on the maximum permitted Linear Heat Generation Rate (LHGR) in fuel rods, depending on rod design and fuel burn-up, during different irradiation modes, e.g.: Steady-State (SST), AOOs, Thermal Transients, Power Ramps, etc. Examples of operational limits for BWR fuel rods are shown in Fig. 1, which are used as Boundary Conditions for the sample calculations, as discussed in Chapter 4.

As mentioned above, a localized excess pre-oxidation of the cladding may, however, alter the operational limits obtained for unaffected fuels, which is the main subject of the current paper.

To begin, the operational limits just mentioned are discussed in more detail below, along with underlying fuel design criteria. Here selected are the limits and design criteria which are basically common for different vendors and countries. Overall, comparison between different fuel types, vendors and countries is beyond the scope of this paper, but can be found elsewhere – for example, in the OECD/NEA report [8]. It is to be noted, that a new calculation methodology, presented in the current paper is deemed to be applicable to different fuel types and reactor conditions (e.g. BWR, PWR and VVER). However, specific calculations are presented in Chapter 4 for just a few selected examples of the operational limits and design criteria of the modern BWR fuel rods, which are expected to be essentially affected by the local oxidation.

2.2. Thermo-Mechanical Operational Limit

A Thermo-Mechanical Operational Limit (TMOL) is the maximum permitted local power in fuel rods during SST irradiation, which is usually presented as a function of fuel burn-up. It is guaranteed that a continuous operation with such hypothesized power history won’t result in violation of any design criteria specified by the vendor for a specific fuel design of interest. Core power distribution is continuously monitored in an NPP, avoiding the real local LHGR to exceed TMOL during normal SST operation. Since a TMOL bounds all rod power histories, experimental and analytical justification of fuel reliability using this TMOL as the Boundary Condition (BC), against appropriate design criteria, is deemed to be valid for all the fuel rods operated in an LWR, unless some parameters of fuel design are changed.

A typical TMOL function for BWR fuel rods was assumed in the current calculation, as shown in Fig. 1 (a red, thick, solid curve). Specifically, the TMOL power history in question has been used for simulating base irradiation of the rods before AOOs, when justifying fuel reliability against corresponding design criteria, such as the one related to local pellet melting (see Section 2.5.1).

It is to be noted, that an assumption of fuel rod being irradiated along the TMOL up to a specified level of burn-up implies a shorter duration of irradiation in terms of time, than irradiation with a realistic power history. For design criteria, dealing with time dependent processes, such as e.g. cladding corrosion (see Section 2.4), a so-called ‘reduced TMOL’ can be used in supplementary calculations. These calculations are to ensure that the use of a nominal TMOL is sufficiently conservative. Besides, as discussed in Ref. [13], a long-term irradiation with a power as high as TMOL can bring out physical phenomena that may be non-representative of, or atypical for current LWR fuel rods operational conditions, such as e.g. high-temperature fuel restructuring and modifications in pellet geometry. Consequently, operation with the reduced-TMOL power history was assumed in the analysis of base irradiation before simulated power ramps, within analysis of the two AOO related design criteria (see Sections 2.5.2 and 2.5.3). The reduced TMOL that was used in the current analysis (see Fig. 1) was obtained as a fraction of the nominal TMOL, such that the duration of irradiation amounted to 40’000 eff. hours, which is realistic for a target peak pellet-averaged burnup of ≈ 50 MWd/kgU.

2.3. Internal gas pressure for cladding lift-off

A fuel design criterion for rod internal pressure (RIP) reads that the rod overpressure (i.e. excess gas pressure in the rod above the coolant pressure) is not to cause pellet-cladding gap opening and growth, which is referred to as cladding lift-off [14]. This criterion stems from the analytical consideration that a reduction of gap conductance may lead to a continuous, lasting increase in fuel temperature, subsequent fission gas release and, eventually, cladding failure.

Usually, fuel vendors have been proving that RIP is lower than a conservative threshold for the onset of cladding lift-off, assuming SST irradiation with the TMOL power history (see Fig. 1). Furthermore, this conclusion can be verified through audit calculations by the regulator and NPP. However, since the RIP threshold just mentioned is derived and verified assuming fuel rods being unaffected, it may need adjustment in the case of rods with an excess local oxidation of the cladding.

2.4. Operational limits for cladding corrosion

The fuel design criterion for cladding corrosion requires that the maximum oxide layer thickness at the outer surface of the cladding does not exceed a design limit that can compromise the rod reliability. The rationale behind this limitation is to mitigate the above-mentioned detrimental effects of the oxidation on mechanical and thermal properties of the cladding. Moreover, waterside cladding oxidation is deemed to be closely correlated with the quantity of hydrogen absorbed by the cladding (see e.g. the MATPRO function CHUPTK [1]), noting that the H-uptake has been currently considered as a crucial parameter for the fuel safety evaluation [16,17].

According to the OECD/NEA Review of Fuel (Safety) Criteria [8], for design purposes, an oxide thickness limit for traditional alloys (e.g. zircaloy) is usually in the range of 100 μm (wall averaged value); this value is taken from post-irradiation examination (PIE)
data at the end of life (EOL) and reasonably bounds experimental data from fuel operated in commercial LWRs. It was however recognized in Ref. [8], that: “unfortunately, the interpretation of these criteria in different countries, and by different fuel vendors, is not unambiguous, e.g. because the cladding region over which the average is taken is often ill defined”.

It is to be noted that, hereinafter, the term ‘oxide thickness’ means the thickness of a metallic cladding converted into the ZrO2. The increase in cladding material volume due to oxidation is not taken into consideration. This suggests that the extra volume of the oxide is assumed to be subject to spalling. Therefore, the same value of oxide thickness was assumed in the current scoping analysis when evaluating mechanical- and thermal-effects of oxidation. However, for more conservative (e.g., licensing) calculations, the assumed effective oxide thickness for thermal effects can be larger than the thickness of oxidized metal, by a factor of up to 1.56 [30], which is the Pilling-Bedworth ratio specifying relative increase in Zirconium volume due to oxidation.

2.5. Operational limits for rod reliability during AOOs

2.5.1. Operational limit for fuel melting

One of the design criteria [8] requires that the centerline fuel temperature always remains below the melting temperature during SST operation and AOOs. A fuel vendor has been determining values of maximum local LHGR, above which the fuel would start melting during a postulated AOO. Eventually, the power limits in question can be verified through audit calculation by the regulator and NPP.

The operational limits for fuel melting, as e.g. shown in Fig. 1, are obtained assuming unaffected fuel rods. Since the excess oxidation of the cladding would result in an increase in cladling- and fuel-temperature, an appropriate adjustment of the current limits for the rods with affected cladding is necessary which would capture detrimental effects of excess pre-oxidation (see Section 4.4.2).

2.5.2. Operational limit for cladding failure due to PCMI

To preclude cladding failure due to PCMI during AOOs, specifically fast power ramps, fuel vendors introduce a design criterion for transient cladding strain. This criterion requires that the total (elastic plus plastic) hoop strain in the cladding due to a postulated fast power ramp cannot exceed a threshold of 1% [15]. A fuel vendor has been determining ramp levels, starting from the SST LHGR, at which the total cladding hoop strain due to a postulated power ramp would reach 1%. Since the excess oxidation of the cladding results in degradation of mechanical and thermal properties of the cladding, an appropriate adjustment of the corresponding limits (see Fig. 1) for the rods with pre-oxidized claddings may be necessary, which would capture detrimental effects of the excessive pre-oxidation (see Section 4.4.3).

2.5.3. Operational limit for cladding failure due to PCI-SCC

After several decades of fuel operation in LWRs, effective measures have been found by vendors and operators, to avoid cladding failure due to Stress Corrosion Cracking (SCC) caused by Pellet-Cladding Interaction [31]. Specifically, no failures by PCI-SCC have been reported since years in BWR fuel rods using barrier claddings (i.e. claddings with the inner Zr-liner) [28]. However, the use of PCI-threshold power for rods with non-barrier claddings is recommended, as a precaution. Exceeding of a PCI-threshold by the local LHGR in a fuel rod during AOOs suggests that an operator (an NPP) is to impose additional constrains on a rate of power increase during corresponding phases of the transients. If the PCI-threshold, as e.g. shown in Fig. 1, was obtained for unaffected fuel rods, the excess oxidation of the cladding would result in degradation of mechanical and thermal properties of the cladding, and appropriate adjustment of the limits would be necessary (see Section 4.4.4).

3. Models and methods used for the analysis

3.1. FALCON model types

The FALCON code [11,12] was created by integration of the capabilities of a code for steady-state fuel rod behaviour analysis (ESCORE) and a fast transient code (FREY). The solution processor of the FALCON code is based on the Finite Element Method (FEM), which allows for fully 2-D thermal and mechanical analysis of fuel rod behaviour under SST and transient irradiation conditions. An advanced method is employed in the code for predicting the cladding failure, considering different mechanisms. Specifically, cladding burst during the Loss of Coolant Accident (LOCA), Stress Corrosion Cracking and pellet-cladding mechanical interaction (PCMI) during the power ramps, are predicted based on the concept of a Cumulative Damage Index (CDI), as well as the calculated spatial distribution of time-dependent stresses, strains and Strain Energy Density (SED).

While providing a robust numerical solver and main models for physical processes and material properties of the fuel and cladding, the FALCON code is flexible enough, allowing users to extend their simulation capability by adding or modifying models and coupling the code with other numerical tools. In particular, the Paul Scherrer Institute (PSI – Switzerland) has been using the FALCON code as the main tool for fuel reliability- and safety-evaluation, as well as a platform for its own method development. For example, the current calculations were performed with the FALCON code [11] coupled to the GRSW-A model [18], which was recently upgraded to Version 4.00 [19]. The GRSW-A model predicts macroscopic variables of fuel state, such as FGR and pellet swelling, based on the analysis of meso- and microscopic processes in each integration point of the pellet mesh [20].

Two different types of finite-element models of the FALCON code were used in the current analysis, referred to as FULL and SLICE-DO model of the FALCON code, Nuclear Engineering and Technology, https://doi.org/10.1016/j.net.2019.07.010
SLICE models (see Fig. 2). Depending on specific goals pursued, the model types in question utilized different physical models and boundary conditions, as specified in Table 1.

FULL models (Fig. 2 — left) utilize the R-Z system of coordinates. Models of this type are used in the most typical problems of integral rod behaviour simulation, with the coupled 2-D calculation of thermal-mechanics, thermal-hydraulics of the equivalent coolant channel associated with a single rod, as well as rod internal pressure (RIP) and evolution of fuel microstructure and fission gas release. The whole irradiation history can be analyzed with FULL models. Also, the calculation can be terminated and resumed at any time-point of simulated irradiation, with a special procedure of the calculation restart [21].

It is to be noted that the use of a FULL type model is a prerequisite for applicability of the built-in thermo-hydraulic model of the FALCON code [11]. The model in question calculates rod-to-coolant heat transfer using a closed channel enthalpy rise model with heat transfer coefficients and critical heat flux correlations like those used in the EPRI RETRAN and VIPRE thermal-hydraulic programs [23,24]. The model can be used by full-length rod models, using an R-Z coordinate system. The analysis is to be fed by the coolant conditions [25] (inlet coolant mass flow rate, temperature, quality, and pressure) and parameter of channel geometry (cladding diameter and effective thermo-hydraulic diameter).

The fully coupled FALCON and GRSW-A analysis was used by the current FULL analysis for calculation of FGR and fuel swelling. The CORROS correlation from MATPRO [1] was used in FALCON for low-temperature cladding oxidation, noting that all the current calculations assumed the oxidation model parameters corresponding to BWR irradiation conditions.

The FALCON code employs the Limbäck-Andersson model for the primary and steady-state cladding creep [22]. This model accounts for the primary and steady-state creep and includes dependencies on time, temperature, stress, and fast-neutron flux, as well as the metallurgical conditions.

Problems analyzed with FULL models deal with axisymmetric, azimuthally uniform distribution of the initial parameters and predicted variables of fuel rod state. In the context of the current study, the FULL models were used for verification of the vendor's results regarding operational limits in unaffected fuel rods, as well as in the analysis of base irradiation of integral rods before the simulated transients.

SLICE models (Fig. 2 — right) utilize the R-θ system of coordinates and are designed for 2-D simulation of local effects, using azimuthally non-uniform, time-varying boundary conditions. These models provide predictions for distribution of the main variables of a thermo-mechanical state (i.e., the stress, strain and temperature) in a selected axial node of the rod during thermal transients that occur in a certain time-point of the simulated irradiation, and their dependents (e.g., the cladding damage index, strain energy density, oxide thickness, etc.). Because analysis with SLICE models is applied to a single axial node of the rod and a certain time-point of irradiation, appropriate initial and boundary conditions must be specified by the user [25], largely, based on analysis of integral rod behaviour with a FULL model, viz.: the initial cladding geometry (particularly, cold gap size in the axial node of interest before the transient), fuel burnup, fast-neutron fluence, as well as the transient histories for local LHGR and fast-neutron flux, internal gas pressure, cladding-to-coolant heat-transfer boundary conditions, etc.

A special model, SLICE-DO (see Table 1), was developed for analysis of fuel behaviour in affected (pre-oxidized) axial nodes of the rods by means of simulating effects of a localized excess-oxide spot on mechanical and thermal properties of the cladding during further operation. The cladding mesh was modified to account for reduced load-bearing thickness of the cladding. Also, the user-specified boundary conditions for the equivalent heat transfer coefficients were defined, through the IRRADIATION-CONVECTION set card in the FALCON input files, to account for the thermal resistance of the oxide spot. The details of the boundary conditions used by this specific model are described in Section 3.2.

Like any SLICE type model, SLICE-DO employs some
simplifications in comparison to the FULL type models. Specifically, an assumption of plane-stress for the axial strain constraint in the fuel stack and cladding, and an engineering model for the steady-state fuel swelling, FSWELL, are used because these are the only options for the corresponding parts of simulation available for SLICE type models of the FALCON code. The FSWELL model of the FALCON code [11] was developed using several data sets, including the Nuclear Fuel Industry Research Program (NFIR) data and EDF UO2 data [26]. This is, basically, an empirical correlation that applies to steady-state (or so-called ‘solid’) swelling of irradiated UO2. Apart from the porosity generated by rim restructuring [27], the FSWELL model does not include simulation of any transient gaseous swelling, which is addressed in a mechanistic GRSW-A model [20] available with FULL models.

It is to be noted, that the nominal operational limits, as defined for unaffected fuel rods (see Fig. 1), have been obtained (or verified, in case they are derived by the vendor) with FULL models, using the mechanistic model, GRSW-A, for fuel swelling. Appropriate analysis was an integral part of a special project conducted at PSI. Detailed discussion of the project just mentioned is beyond the scope of the current paper. However, it should be emphasized, that due to a relatively short (60 s) duration of the simulated power ramps, the predicted contribution of transient gaseous swelling at RTL not exceeding ~10%. Although, contribution of the transient swelling was shown to increase with fuel burn-up, particularly, when the fuel stack is.

In consideration of the above-mentioned simplifications, and in compliance with the established methodology of application for SLICE models [29], the SLICE-DO model was used, largely, to assess a relative enhancement of the selected figures of merit (for example, peak values of cladding stress, strain, CDI, SED, creep-out rate, or centerline fuel temperature, etc.) due to the simulated perturbation of a single boundary condition, such as e.g. a localized excess oxide spot due to redundant waterside corrosion. In general, the estimated relative enhancement, just mentioned, can be further used for introducing appropriate corrections into the nominal numerical solutions (i.e., the operational limits of unaffected rods), which are obtained with the FULL models. In order to avoid a build-up of uncertainty, associated with the simplifications just mentioned, the SLICE-DO model can be employed in thermal-mechanical analysis of relatively short periods of irradiation, such as power ramps, unless the analyzed processes are expected to be independent on the simplifications in question.

Within the current study, the SLICE-DO model was employed for calculation of the low-temperature oxidation in an affected axial node of the rod, and the enhancement in the cladding creep rate for adjustment of the lift-off RIP limit, noting that these calculations were not affected by the above mentioned simplifications. Furthermore, the SLICE-DO model was used in calculation of power ramps, in relation to the fuel design criteria related to fuel melting and cladding failure due to PCMI and PCI assisted Stress-Corrosion Cracking (PCI-SCC).

### 3.2. The SLICE-DO model for simulation of affected axial node behaviour

To simulate the effects of localized excessive pre-oxidation on fuel rod behaviour during further incident-free SST irradiation and AOOs, mutual thermal and mechanical impact of the affected cladding area was modelled, as shown in Fig. 3. Presented in Fig. 3 is the outermost layer of the cladding finite element mesh (not to be scaled), corresponding to an axial position where the affected cladding is.

The mechanical effect, due to reduction of the load-bearing (metallic) cladding thickness, is simulated by modifying radial co-ordinates of the cladding nodes, in accordance with the initial sizes of the excess oxide spot: the thickness (δ), and the angular half-size (θ₀/2). Thus, the radial co-ordinates of the outer surface nodes in the modified cladding mesh correspond to the position of the metal-to-oxide interface in a real, affected cladding. This modification of the cladding mesh, alone, would be sufficient for considering cladding state e.g. after the oxide spallation.

The thermal effect is due to a relatively low thermal conductivity of the zirconium oxide, which was calculated using the ZOTCON correlation from MATPRO [1]

\[
\lambda = A + BT
\]

where A and B are the model constants, T the temperature.

The thermo-hydraulic boundary conditions for FALCON calculation with the SLICE-DO model need to be input, such that the temperature in the outermost nodes of the modified mesh equal
the temperature of the metal-to-oxide interface in the affected (e.g. pre-oxidized) axial node of the rod. First, cladding outer surface temperature, \( T_{\text{cos}}(z; \theta = Z_{\text{DO}}) \), in a selected axial position \( Z_{\text{DO}} \), during entire irradiation period of interest is calculated by FALCON using the FULL model, with the built-in coolant enthalpy rise model. Next, the FALCON analysis for the affected axial node during the same irradiation period is performed using time-dependent input values, BULKTEMP and FILMCOEF [25], such that:

\[
T_0(z = Z_{\text{DO}}; t) = \text{BULKTEMP} + \frac{\Phi}{\text{FILMCOEF}}
\]

(2)

where \( T_0 \) is the temperature at the metal-to-oxide interface, BULKTEMP the user input function for external bulk temperature, FILMCOEF the user input function for equivalent heat transfer coefficient, \( \Phi \) the heat flux density through the outer cladding surface.

The heat flux density through the outer cladding surface, \( \Phi \), is calculated internally by the FALCON code, based on 2-D analysis of the heat generation and transport in the fuel rod slice, and the user input for Linear Heat Generation Rate (LHGR) and Thermo-Hydraulic Boundary Conditions (BULKTEMP and FILMCOEF).

The user input for external bulk temperature, BULKTEMP, in the SLICE-DO model is assumed to be equal to \( T_{\text{cos}}(z; \theta = Z_{\text{DO}}) \), as calculated with the FULL model after the first FALCON run just mentioned:

\[
\text{BULKTEMP} = T_{\text{cos}}(z = Z_{\text{DO}})
\]

(3)

The time- and azimuthal-position-dependent values for the equivalent heat transfer coefficients, FILMCOEF, are calculated based on the azimuthal profile of the initial oxide thickness in the pre-oxidized axial node:

\[
\text{FILMCOEF} = h_{\text{eff}} - \frac{Z}{\delta} = \frac{1}{\delta} \left[ A + B \left( T_{\text{cos}} + \frac{\Phi'}{\lambda(T_{\text{cos}})} \frac{\delta}{Z} \right) \right]
\]

(4)

where \( \delta \) is the local oxide thickness, \( Z \) the layer-averaged thermal conductivity of the zirconium oxide, \( \lambda(T_{\text{cos}}) \) the oxide thermal conductivity at a temperature of the outer cladding surface.

The heat flux density, \( \Phi' \), on the right-hand side of the approximated Eq. (4) is assessed under the assumptions of azimuthally uniform, steady-state distribution of temperature and heat flux in the rod slice considered:

\[
\Phi' = \frac{\text{LHGR}}{\pi D}
\]

(5)

where LHGR is the linear heat generation rate in the analyzed axial node of the rod, \( D \) the cladding outer diameter. Note that calculational uncertainty due to the assumptions just mentioned is relatively low, because Eq. (1) shows up rather low sensitivity of the thermal conductivity of the zirconium oxide to temperature.

The case specific values for FILMCOEF and BULKTEMP were input for all the outer nodes of the modified cladding mesh, as shown in Fig. 3, through corresponding set cards of the THERMAL command card in FALCON input files [25]. The nodes were divided into groups with equal oxide thickness (\( \delta \) in the affected sector, and zero in the unaffected sector). The node grouping was implemented through the IRRADIATION-CONVECTION set card of the MODEL command card.

The SLICE-DO model with the above specified boundary conditions allows for evaluation of temperature distribution in the claddings and pellets in affected axial nodes of fuel rods during further irradiation, e.g. power ramps. For example, shown in Fig. 4 are the results of calculation using FALCON with the SLICE-DO model for distribution of temperature in a fuel rod slice assuming extra thermal resistance at the outer cladding surface as equivalent to a 300 \( \mu \)m thick oxide spot with an angular half-size of 40\(^\circ\). Presented in Fig. 4 are the variable distributions at a Ramp Terminal Level (RTL) of 40 kW/m.

Fig. 3. Finite-element model schematics for simulation of locally pre-oxidized axial node behavior

Note: The ‘unaffected’ mesh is shown with black nodes. The nodes with modified coordinates are shown in red. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Fig. 4. Examples of calculated temperature distribution in cladding (top) and mid-radius pellet zone (bottom). Presented are the variable distributions at a Ramp Terminal Level of 40 kW/m.
Apart from a direct effect on thermal expansion of the pellets due to increase in fuel temperature, aggravation of the mechanical cladding state can be caused by the significant influence of temperature on the mechanical cladding properties at working conditions (i.e. under the base irradiation and A0Os), such as creep rate and yield strength. Moreover, localized non-axisymmetric distribution of an affected cladding area can also amplify local cladding strain, Strain Energy Density (SED) and Cumulative Damage Index (CDI), caused by PCMI during power ramps, due to thermal-mechanical concentration, viz.: fast localized cladding creep or plastic deformation, along with stress relaxation in the overheated part of the cladding, against reduced strain in the unaffected part due to higher resistance to permanent deformations (creep and plasticity) at a lower temperature (see Fig. 5).

For example, as shown in Fig. 5 (top), accounting for the effects of local overheating on cladding properties resulted in an increase in calculated peak local hoop strain during the power ramp, by a factor of ~3 - 4, compared to the hoop strain in the unaffected part of the cladding. Consequently, accounting for such effects could result in violation of fuel rod design criteria (see Chapter 2) for cladding failure due to PCMI or PCI-SCC and, eventually, prediction of the cladding failure in the affected rod during real operation.

The developed capability allowed for analysis of the entire 180-degree symmetry sector of the rod slice. It is to be noted that, in general, simulations of the mechanical and thermal effects of an excess-oxide spot are effectively de-coupled in the SLICE-DO model. This allows for modeling a mutual effect, as well as separated mechanical- (e.g., local oxide spot spallation) or thermal- (e.g., a thermal barrier due to a local spot of crud) effects.

4. Results and discussion

4.1. Parameters of rod design and operational conditions

The current scoping analysis assumed the specifications for modern BWR fuel rods [28], as had been used in a previous study [13]. The main parameters of fuel rod design and irradiation conditions, as assumed in the current calculations, are specified in Table 2.

Parametric studies with the SLICE-DO model were carried out with a view of exploring the influence of local excess oxide sizes (the angular size and the thickness) on the predicted variables of the fuel rod state. The scoping analysis of the response to power transients was limited to two arbitrary cases of affected rods. The cases in question were characterized by the two postulated values for a local excess-oxide thickness, as specified in Table 3.

4.2. Cladding lift-off

As mentioned above, excessive local oxidation results in an increase in cladding temperature and reduction of its effective, mechanical-load bearing thickness. The latter also suggests an immediate increase in tensile hoop stress in an over-pressurized
cladding, with the rod internal pressure (RIP) higher than the external coolant pressure. Therefore, enhanced oxidation will lead to an increased creep-out rate in the affected cladding areas due to over-pressurization.

Presented in Fig. 7 are the results of calculation for creep-out strains in affected- and unaffected-claddings at exposure to a time-constant overpressure, assuming rod internal pressure being equal to the lift-off limit, \( RIP = P_{\text{lift-off}} \). The primary and secondary creep-out of unaffected- and affected-claddings was calculated with the SLICE-DO model, using the Spot-MT boundary conditions (see Table 1). The cladding creep-out in a contact-free rod slice was calculated using the Limb-Andersson model [22].

The angular half-size of the excess-oxide spot, \( \theta_{\text{DO}}/2 \), assumed in the calculation as shown in Fig. 7 was 30°. The oxide thickness in a pre-oxidized cladding corresponded to affected rods from Case 2 (see Table 3). For the affected cladding, presented are the azimuthally averaged strain, and the local strains in the coldest and the ‘coldest’ nodes of the slice, corresponding to angular coordinates \( \theta = 0° \) and \( \theta = 180° \), respectively. An SST creep-out rate was considered as a figure of merit, which was defined at a simulated time of 1000 h after application of the overpressure. The azimuthally averaged creep rates were defined from calculated distribution of the cladding hoop strain in the cladding symmetry sector during the simulated period, using Eq. (6):

\[
\hat{\varepsilon}_{\text{DO}} = \frac{1}{\pi} \int_0^{\pi} \hat{\varepsilon}(\theta) \, d\theta
\]

where \( \hat{\varepsilon}(\theta) \) is the calculated azimuthal distribution of the hoop strain in the inner elements of the cladding for the 180-degree symmetry sector of the slice.

Significant enhancement of the creep rate on the affected side of the cladding can be seen in Fig. 7. As a counter-measure, a reduction of the lift-off RIP limit for affected rods was proposed, in comparison to the one established by the vendor for unaffected rods, which would capture the effect of excessive oxidation on the cladding creep-out rate. The following condition was accepted for definition of the adjusted RIP limit, \( P_{\text{adj}} \):

\[
\hat{\varepsilon}_{\text{U}} \left( RIP = P_{\text{lift-off}} \right) = \hat{\varepsilon}_{\text{DO}} \left( RIP = P_{\text{adj}} \right)
\]

where \( RIP \) is the rod internal pressure assumed in the calculation, \( \hat{\varepsilon}_{\text{U}} \) the creep-out rate calculated for unaffected cladding, \( \hat{\varepsilon}_{\text{DO}} \) the azimuthally averaged creep-out rate calculated in the inner layer of elements of the affected cladding, \( P_{\text{lift-off}} \) the established RIP limit for the onset of lift-off in unaffected rods, \( P_{\text{adj}} \) the adjusted RIP limit for affected rods.

Adjusted RIP limits were defined for different angular sizes of excess-oxide spots, assuming an affected rod from Case 2 (see Table 3). To this end, the calculated azimuthally averaged creep-out rates were plotted for the range of RIP from the external coolant pressure \( P_{\text{coolant}} \) (7.3 MPa) to the lift-off limit, \( P_{\text{lift-off}} \), in unaffected rods, as shown in Fig. 8. A postulated, conservative value of 15 MPa was assumed in the current scoping calculation for the lift-off limit, \( P_{\text{lift-off}} \).

The adjusted lift-off pressure limits were determined graphically and presented in Fig. 9. The highest effect was, explicity, predicted for the axisymmetric excess pre-oxidation (\( \theta_{\text{DO}}/2 = 180° \)), for which the adjusted lift-off RIP turned out to be nearly 30% lower than the unaffected value.

### 4.3. Cladding oxidation

Temperature redistribution in a locally pre-oxidized cladding will affect the growth of oxide layers during further irradiation. It is to be noted that a localized pre-oxidation can reduce the rate of oxide propagation during further irradiation, in comparison to uniformly distributed initial oxidation, due to redistribution of the heat flux and temperature in the cladding. For example, Fig. 10 shows azimuthal profiles of the oxide thickness in a fuel rod slice after the same irradiation, as calculated for different angular sizes assumed for the initial oxide spot. The mitigating effect is particularly pronounced for the small sized spots. The effect levels out with the increase in initial angular size.

---

**Table 2**

<table>
<thead>
<tr>
<th>Parameter, unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel rod type</td>
<td>BWR 10 × 10 (Full Length Rod)</td>
</tr>
<tr>
<td>Fuel material</td>
<td>Enriched UO₂</td>
</tr>
<tr>
<td>Cladding material</td>
<td>Zircaloý-2</td>
</tr>
<tr>
<td>Cladding yield strength (YS), MPa</td>
<td>MATPRO⁹</td>
</tr>
<tr>
<td>Coolant pressure at inlet, MPa</td>
<td>7.3</td>
</tr>
<tr>
<td>Coolant temperature at inlet, °C</td>
<td>289</td>
</tr>
</tbody>
</table>

* Yield Strength was calculated internally by FALCON using the CMLIMT model of MATPRO [1].

**Table 3**

<table>
<thead>
<tr>
<th>Parameter, units</th>
<th>Classification of affected rods</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Case 1</td>
</tr>
<tr>
<td>Base (uniform) oxide thickness on the unaffected side of the cladding, μm</td>
<td>20</td>
</tr>
<tr>
<td>Additional local oxide thickness on the affected side of the cladding (Δ), μm</td>
<td>70</td>
</tr>
</tbody>
</table>

---

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4.4. Fuel rod behaviour during AOOs

4.4.1. Consistent simulation of base irradiation and power ramps

Effects of excess local oxidation on variables of a fuel rod state during AOOs were explored using the SLICE-DO model of the FALCON code. In general, this calculation addressed pre-oxidation stipulated enhancement in appropriate figures of merit, as selected for the appropriate design criteria (see Section 2.5), in comparison to the case without excessive pre-oxidation.

In all the cases, the transient analysis with the SLICE-DO model was preceded by a calculation of base irradiation of the full-length rod. To this end, the FULL model was utilized. The calculation of base irradiation yielded parameters of the fuel rod state in a challenging, peak-power axial node of the rod just before the AOO, which were used as initial conditions for the transient analysis, viz.:

- Fast-neutron fluence;
- Cold-gap ratio. This is an input parameter of the FALCON code — particularly important when applying SLICE type models, which is defined as a ratio of the pellet-cladding gap size (at room temperature) before the transient to the as-fabricated gap-size. The selected value adjusts pre-transient gap size to the value obtained from calculation of the base irradiation of the full-length rod;
- Initial rod internal pressure (RIP) and gas composition;
- Uniform (axisymmetric) component of the initial oxide thickness.

4.4.2. Power limit for fuel melting

Peak local fuel temperature in a challenging axial node was calculated during a simulated, relatively fast linear increase in LHGR, starting from the level of base irradiation (i.e. the TMOL power), to a specified operational limit for fuel melting at the level of burnup considered (see Fig. 11). Hereinafter, a ‘challenging axial node’ means the peak power position of the rod with assumed excessive local oxidation of the cladding. The SLICE-DO model was used. Comparative calculation with the same model was performed assuming unaffected cladding (without pre-oxidation), and affected cladding with oxide thickness corresponding to rods from Case 1 and Case 2, as specified in Table 3.

Various

Fig. 8. Calculated azimuthally-averaged rate of SST cladding creep as function of RIP.

Fig. 9. Calculated normalized RIP limit for the onset of cladding lift-off as function of angular half-size of the excess-oxide spot for affected rods from Case 2.

Fig. 10. Calculated azimuthal profile of the oxide layer thickness after steady-state irradiation assuming different initial oxide-spot sizes.

Note: The assumed initial oxide thickness was 30 μm in the affected (pre-oxidized) part of the cladding (θ_0 < θ < θ_0/2) and zero in the unaffected part.
angular half-sizes of an excess-oxide spot were considered, ranging from 0° (no excess oxidation) to 180° (axisymmetric excess oxidation).

The adjusted power limits for fuel melting were defined, as functions of pellet burn-up, for affected rods from Case 1 and Case 2, considering different angular sizes of the excess oxide spot. The obtained functions revealed decreasing dependency on the excess oxide thickness and angular size, with the minimum being predicted for the axisymmetric pre-oxidation (θDO/2 = 180°). The results of calculation for the axisymmetric pre-oxidation (i.e. conservative) case are presented in Fig. 12. As seen in Fig. 12, excess pre-oxidation of the cladding in rods from Case 2 can result in a relative reduction of the ‘melting power’ by ~4–8%.

4.4.3. Ramp level limit for cladding failure due to PCMI

The peak local hoop strain of the cladding in a challenging axial node was calculated, with the SLICE-DO model, during a simulated relatively fast linear increase in LHGR, starting from the level of base irradiation (i.e. 10% of the TMOL power) to a predetermined design limit for PCMI failure at several burnup levels. Comparative calculation with the same model was performed assuming unaffected cladding (without pre-oxidation), and for the excess oxide thickness corresponding to affected rods from Case 1 and Case 2, as specified in Table 3. Various angular half-sizes of an oxide spot were considered, ranging from 0° (no defect) to 180° (axisymmetric excess oxidation).

The calculated peak cladding hoop strains were plotted, as function of LHGR, as e.g. shown in Fig. 13. Graphical processing of the obtained diagrams allowed for determining adjusted LHGR limits for precluding PCMI failure in affected axial nodes, for different levels of burnup and defect sizes.

Explicably, for the same burnup, the calculated peak local hoop strain increases, and the adjusted PCMI power limit decreases with an increase in excess oxide thickness, as shown in Fig. 14. The predicted dependency of peak local hoop strain on angular half-size of the excess oxide spot is not straightforward, usually showing the maximum in the hot-spot, where the localized pre-oxidation is (see Fig. 15). The reason of this prediction is the concentration of the cladding strain in a ‘weaker’ (hotter and thinner) part of the slice, as mentioned in Section 3.2 (see e.g. Fig. 5 - top).

The normalized PCMI limits for power ramp levels in affected and unaffected rods are shown in Fig. 16. Presented in Fig. 16 are the conservative (i.e. the lowest) values obtained from the calculation.
for different angular sizes of the excess oxidation spot, noting that at a burnup higher than ~30 MWd/kgU, the lowest values were predicted for localized pre-oxidation with $\theta_{DO}/2 \approx 30^\circ$. It can be seen from Fig. 16, that excess pre-oxidation of the cladding in rods from Case 2 can result in a relative reduction of the PCMI operational limits by ~20–40%.

4.4.4. Power limit for cladding failure due to PCI-SCC

In compliance with the previous special study [29], the current calculation used peak local values of the hoop stress and cumulative damage index (CDI) in a cladding as figures of merit for analysis of cladding failure due to PCI-SCC.

Fig. 15. Calculated azimuthal profiles of local hoop strain in a pre-oxidized slice at RTL for different angular sizes of oxide spot.

Fig. 16. Normalized ramp level limits (conservative) for PCMI cladding failure in affected and un-affected rods.

Fig. 17. Series of power transients as simulated for definition of adjusted PCI-threshold in affected fuel rods.

Fig. 18. Examples of calculated peak local CDI (top) and hoop stress (bottom) for simulated series of power transients.

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The variables in question were calculated, with the SLICE-DO model, for a challenging axial node of the rod during assumed, relatively slow power transients. A sample normalized local power history during a BWR cycle start-up was used as the appropriate boundary condition for this calculation. Series of power ramps, starting from the level of base irradiation (i.e. 10% of the TMOL power), were considered assuming different values of the ramp terminal level (RTL), followed by a sufficiently long periods of power conditioning, as shown in Fig. 17. The duration of power conditioning of 100 h was assumed in the calculation, which ensured saturation of the increase in CDI during simulated transients. Examples of calculated hoop stress and CDI, corresponding to the power histories shown in Fig. 17, are shown in Fig. 18.

The calculated maximum values of peak local CDI and hoop stress, as reached during the simulated transients were defined and plotted as functions of RTL, as shown in Fig. 19. Graphical processing of the obtained diagrams allowed for determining adjusted PCI-thresholds for precluding PCI-SCC failure in the affected axial nodes of the rods.

A special sensitivity study revealed that the maximum enhancement in peak local CDI and hoop stress and, correspondingly, the minimum values for the adjusted PCI-threshold were predicted for relatively small angular half-sizes of the pre-oxidation spots, \( \theta_{\text{pool}} = 10^\circ \). The reason of this prediction is the above-mentioned effect of thermal-mechanical concentration in a ‘weaker’ (hotter and thinner) part of the cladding.

Conservative (i.e. the lowest predicted) values of the adjusted PCI-threshold, which would capture the pre-oxidation stipulated enhancement in both CDI and hoop stress, were defined for different levels of burn-up, for affected rods from Case 1 and Case 2. These results are presented in Fig. 20. It is to be noted, that up to a burnup of \( \approx 20 \text{ MWd/kgU} \), an absent or weak pellet-to-cladding mechanical contact was predicted during the transients considered. Consequently, no adjustment of the original PCI-threshold was found necessary for burnup values below 20 MWd/kgU. For burnup higher than 20 MWd/kgU, excess pre-oxidation of the cladding in rods from Case 2 was shown to result in a relative reduction of the PCI-threshold power by up to \( \approx 35\% \).

5. Conclusions

A methodology has been developed, using basic capabilities of the FALCON code, for evaluation of the effects of excessive localized oxidation of the cladding on fuel rod reliability and safety. The key element is a special finite-element model, SLICE-DO, which simulates mechanical and thermal impact of an azimuthally non-uniform pre-oxidized area of the cladding, due to reduction of its mechanical-load bearing thickness and additional thermal resistance at the outer cladding surface. The model allows for numerical simulation of the mechanical response and temperature redistribution in the claddings and pellets in affected axial nodes of fuel rods during further irradiation, such as e.g. power ramps.

Apart from the direct effect on thermal expansion of the pellets due to increase in fuel temperature, aggravation of the mechanical cladding state was predicted due to effects of temperature on mechanical properties of the cladding, such as the creep rate and yield strength. Moreover, localized non-axisymmetric distribution of the affected cladding area was shown to be able to amplify local cladding strain and Cumulative Damage Index (CDI), as caused by Pellet-Cladding Mechanical Interaction (PCMI) during power ramps, due to thermal-mechanical concentration, viz.: fast
localized cladding creep or plastic deformation along with stress relaxation on the overheated side of the cladding, against reduced strain on the unaffected side due to higher resistance to permanent deformations (creep and plasticity) at a lower temperature. Consequently, accounting for such effects with the proposed method is able to explain some unexpected cladding failures.

The methodology was employed for adjustment of selected operational limits, to capture effects of localized oxidation. Specifically, the rod internal pressure for the onset of cladding lift-off was reduced, depending on initial excess oxidation spot sizes. Also, the power limits for Anticipated Operational Occurrences, which are to preclude fuel melting, and cladding failure due to PCMI or Pellet-Cladding Interaction (PCI) assisted Stress-Corrosion Cracking (SCC) were adjusted, accordingly.

The new methodology can be used in fuel behaviour analyses for reliability assessment of re-utilized pre-oxidized rods.

**Declarations of interest**

None.

**Acknowledgement**

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**Appendix A. Supplementary data**

Supplementary data to this article can be found online at https://doi.org/10.1016/j.net.2019.07.010.

**References**


