European Commission

JRC TECHNICAL REPORTS

Development of M5 Cladding Material Correlations in the TRANSURANUS Code

Revision 1

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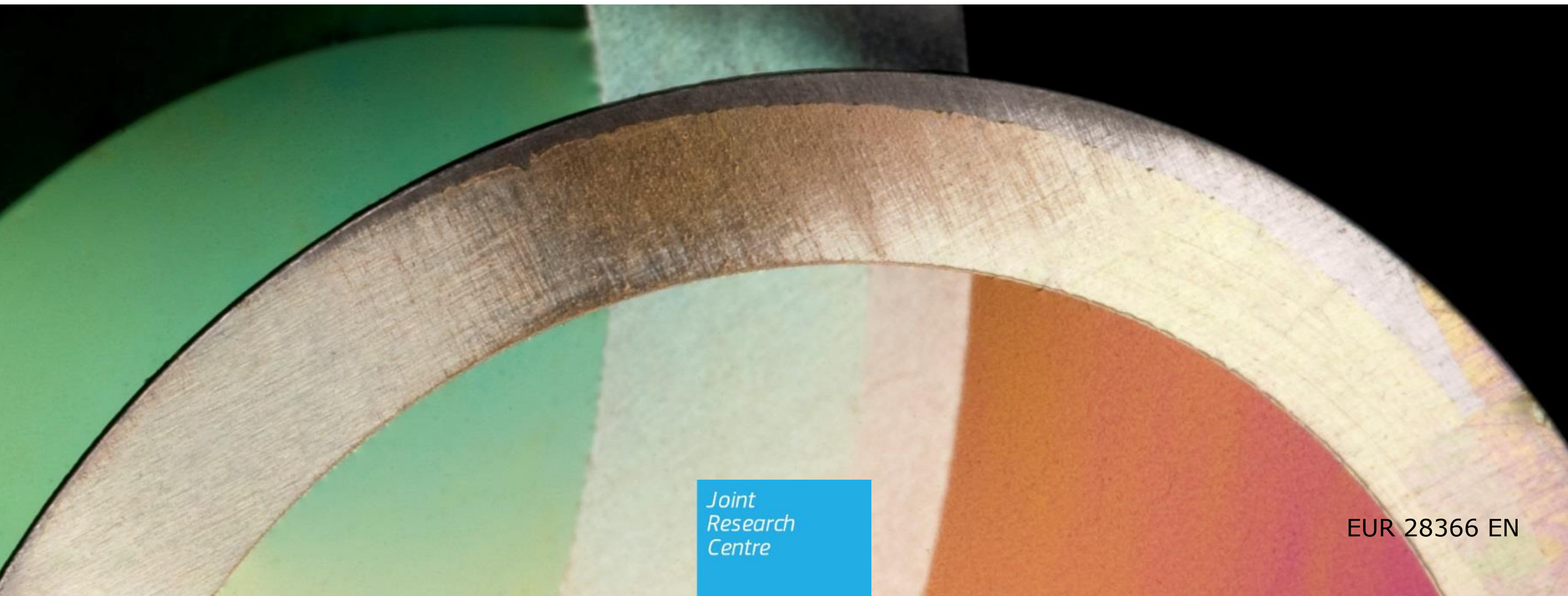
2016



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JRC Science Hub
https://ec.europa.eu/jrc

JRC100644

EUR 28366 EN

PDF	ISBN 978-92-79-64655-3	ISSN 1831-9424	doi:10.2789/320793
Print	ISBN 978-92-79-64656-0	ISSN 1018-5593	doi:10.2789/332092

Luxembourg: Publications Office of the European Union, 2016

How to cite this report: Kecek, A., Tuček, K., Holmström, S., van Uffelen, P., *Development of M5 Cladding Material Correlations in the TRANSURANUS Code: Revision 1*, EUR 28366 EN, Publications Office of the European Union, Luxembourg, 2016, ISBN 978-92-79-64655-3, doi:10.2789/332093, JRC100644.

Contents

Abstract

The technical report is based on an earlier research on material properties of the M5 structural material. Complementing this research with new M5 data found in open literature, a set of correlations has been developed for the implementation to the TRANSURANUS code. This includes thermal, mechanical, and chemical (corrosion) properties of M5. As an example, thermal capacity and burst stress correlations have been proposed using the available experimental data.

The open literature provides a wide range of experimental data on M5, but for some quantities they are not complete enough to be suitable for the implementation to the TRANSURANUS code. A balanced consideration of similarity of M5 characteristics to those of Zircaloy-4 (Zry-4) or E110 have therefore led to the recommendation to use some of these data selectively also for M5. As such, creep anisotropy coefficients of E110 are recommended to be used also for M5.

1. Introduction

The TRANSURANUS code is a computer code for thermal and mechanical analysis of nuclear fuel rods/pins. The code is developed by European Commission's Joint Research Centre (JRC).

In the field of thermal analysis, TRANSURANUS allows a calculation of steady state and transient processes including phase changes. The calculations are solved by an advanced numerical solution technique, which excels by speed and stability. The mechanical analysis is based on constitutive equations assuming an equilibrium state. The solution is based on a superposition of one-dimensional radial and axial mechanical analyses. This concept leads to a semi-analytical problem, which is solved by an effective numerical algorithm. The physical analysis takes in account all relevant phenomena, i.e., thermal and irradiation induced swelling, plasticity, pellet cracking, formation of central void, etc. TRANSURANUS currently allows analyses of all fuel rod types under normal, off-normal and accidental conditions using deterministic and probabilistic principles. The time scale of investigated problems varies from milliseconds to years.

The development presented in this report concerns the assessment and incorporation of thermal (chapter 3), mechanical (chapter 4), and corrosion (chapter 5) properties of M5 advanced cladding material into the TRANSURANUS code.

M5 alloy is a proprietary variant of zirconium alloy with 1% niobium developed by AREVA (cf. Table 1). It is used for fuel rod cladding and structural components (intermediate grids and guide tubes) for all AREVA pressurized water reactor (PWR) designs. M5 has fully re-crystallized microstructure, contains no tin, and has controlled oxygen, iron and sulphur contents. This results in significantly improved in-core corrosion resistance and hydrogen pickup rates compared to Zircaloy-4 alloy, with controlled irradiation induced swelling, and creep behaviour. The alloy is therefore particularly suited for higher duty operating environments (higher burn-up and uprates) of current PWRs (AREVA 2011).

Table 1 Composition of M5 compared to Zircaloy-4 (Zry-4) and E110 alloys. RXA = Fully Recrystallized Alloy; CWSR / SRA = Cold Worked Stress Relieved / Stress Relief Annealed alloy.

Alloy	Sn [wt.%]	Nb [wt.%]	O [wt.%]	Fe [wt.%]	Cr [wt.%]	Ni [wt.%]	Zr	Structure	Phase transformation [K]
M5	--	1.0	0.135 (0.118-0.148)	0.038 (0.015-0.037)	--	--	Bal.	RXA	1023 - 1233
Zry-4	1.45 (1.2-1.5)	--	0.125 (0.09-0.16)	0.21 (0.18-0.24)	0.10 (0.07-0.13)	--	Bal.	CWSR[1]	1080 - 1270
E110	--	1.0	0.060	0.009	--	--	Bal.	RXA	1070 - 1180

The information given in this report is based on the TRANSURANUS code version v1m1j14, which is currently available at JRC Petten.

[1] Sometimes also used in its fully recrystallized condition (RXA).

2. Development of M5 data correlations

The present work complements the previous internal JRC study on material properties of M5 available in open literature. This study considered a full set of thermal, mechanical, and corrosion properties of M5.

Note that although an earlier assessment of M5 cladding properties for the implementation to TRANSURANUS had already been done at TÜV Nord, these implementations are not part of this report and they are a property of Nuclear Power Plants and fuel vendors. In this context, TÜV Nord work concentrated specifically on a creep anisotropy, plastic strain rate (during loss-of-coolant accident conditions), and burst stress of M5.

On the basis of the previous JRC study and new data on M5 behaviour found in open literature, considering at the same time consistency and completeness of these data as well as phenomenological similarity of some characteristics of M5 to those of Zry-4 and E110, a set of material correlations has been developed for the implementation in the TRANSURANUS code.

The proposed correlations are implemented in TRANSURANUS under data property number 21 for the best estimate and 22 for conservative material properties. In case of the corrosion model, data property numbers 38 and 39 are used to describe normal/operational state and high temperature/accidental corrosion behaviour, respectively[2].

The ordering of the sections in this report corresponds to that of the TRANSURANUS Handbook (JRC-ITU 2014).

[2] NB. The definitive allocation of numbers for M5 will be fixed at the later stage when the TRANSURANUS code is updated and some old (unused) material properties are removed.

3. Thermal properties

3.1 Emissivity

The emissivity of fuel cladding is calculated by the EMISS subroutine. TRANSURANUS includes three correlations (no. 19, 20 and 25), but all of them predict the same value of 0.8 (JRC-ITU 2014).

3.1.1 Analysis

On the basis of the review of data available in open literature (Mitchel et al. 2000) the constant emissivity of 0.8 is also proposed to be adopted for the M5 cladding material.

3.1.2 Conclusion

The radiation is not expected to be the most important heat transfer effect. The constant emissivity value is therefore expected to be an appropriate choice.

3.1.3 Draft Correlation – EMISS

```
 221   continue
!      M5 alloy
      emiss = Random_Var(18,4,4)*0.8
      return
```

3.2 Density

Material density is calculated in the subroutine RO. The TRANSURANUS code considers two correlations for density, namely for LWR (no. 20) and VVER (no. 25) cladding materials (JRC-ITU 2014).

3.2.1 Analysis

Both existing LWR and VVER correlations are defined as a constant value and density decrease with increasing temperature is simulated by the multiplication by a factor of eta123, which describes the material strain (dilatation) effect.

As regards M5, based on the review of the available data, it is proposed to choose its density as 6500 kg/m^3, following the modelling approach adopted in the COPERNIC code (FRAMATOME 2004). Comparison of all mentioned density values is given in Table 2.

Table 2 Density of M5, E110 and LWR claddings (JRC-ITU 2014), (FRAMATOME 2004)

Correlation	Value
Proposed M5 correlation	6500 kg/m^3
LWR correlation no. 20	6550 kg/m^3
VVER correlation no. 25	6550 kg/m^3

3.2.2 Conclusion

The proposed M5 density correlation is in a good agreement with already existing TRANSURANUS correlations. Similarly to the existing modelling approach, the proposed correlation adopts a constant value of density, which is then multiplied by a factor taking into account the material dilatation effect.

3.2.3 Draft Correlation – RO

```
 222   continue
!      M5 alloy
!      density in g/mm3 = 0.0065
!      =======
       ro = 0.0065 * eta123 * Random_Var(14,4,4)
       return
!      ++++++
```

3.3 Solidus Liquidus Melt Temperature

In the TRANSURANUS code, the subroutine SOLIMT calculates the cladding melting temperatures. The correlations are given in the code for LWR (no. 19 and 20) and E110 (no. 25) cladding materials (JRC-ITU 2014).

3.3.1 Analysis

In all the existing TRANSURANUS correlations it is assumed that the solidus and liquidus temperatures are the same.

Table 3 Solidus liquidus melt temperatures given by correlations corresponding to LWR, E110, and M5 (JRC-ITU 2014), (Cazalis et al. 2005)

Correlation	Value
Proposed M5 Correlation	2128.15 K
LWR Correlations no. 19 and 20	2098 K
VVER Correlation no. 25	2133 K

Regarding M5, it was decided to use the same temperatures for solidus and liquidus both in the FRAPCON (Luscher et al. 2011) and COPERNIC (Cazalis et al. 2005) codes. The recommended temperatures for M5 are 2133.15 K and 2128.15 K, as given in the FRAPCON and COPERNIC codes, respectively. In TRANSURANUS, it is proposed to use for M5 a conservatively lower value of 2128.15 K from the COPERNIC code, cf. Table 3.

3.3.2 Conclusion

As discussed above, all materials exhibit very similar or same behaviour as regards the solidus/liquidus melt temperature. The difference between the considered values is small (in comparison to absolute values) and this topic probably does not need further detailed research or development.

3.3.3 Draft Correlation – SOLIMT

```
 222   continue

!      M5 alloy
!      data from the COPERNIC code (2128.15)
!      solidus = liquidus

       tmsolk = Random_Var(16,4,4)*(2128.15)
       tmliqk = tmsolk

       return
!      ++++++
```

3.4 Heat of Melting

In the TRANSURANUS code, the subroutine FH calculates the heat of melting. Currently, there are three different correlations implemented in TRANSURANUS: LWR (no. 20), MATPRO-based (no. 19), and VVER (no. 25).

3.4.1 Analysis

The LWR and VVER correlations predict the same constant value for heat of melting equal to 252 kJ/kg. The MATPRO-based correlation predicts the heat of melting as being equal to 225 kJ/kg (JRC-ITU 2014), cf. Table 4.

Based on the recommendation given in (Luscher et al. 2011) it is proposed to use for M5 a constant value of 210 kJ/kg, providing thus conservative estimate when considering heat-up transients.

Table 4 Heat of melting given by correlations corresponding to LWR, E110, and M5 (JRC-ITU 2014), (Luscher et al. 2011)

Correlation	Value
Proposed M5 Correlation	210 kJ/kg
LWR Correlation No. 20	252 kJ/kg
VVER Correlation No. 25	252 kJ/kg
MATPRO-based Correlation No. 19	225 kJ/kg

3.4.2 Conclusion

The proposed M5 correlation is close to the existing MATPRO-based TRANSURANUS correlation. Future development may be aimed at determining a more accurate value.

3.4.3 Draft Correlation – FH

```
 221  continue

!      M5 alloy
!      Data from FRAPCON
       fh = 210. * Random_Var(17,4,4)
       return
!      ++++++
```

3.5 Thermal Strain

Thermal strain calculations are performed in the TRANSURANUS code in the subroutine THRSTRN. Each thermal strain component (axial, radial, and tangential) is treated separately. TRANSURANUS includes thermal strain correlations for LWR (no. 20) and VVER (no. 25) conditions, as well as from MATPRO (no. 19) (JRC-ITU 2014).

3.5.1 Analysis

The thermal strain correlation for E110 is rather simplified since it does not take the phase transition into account. The strain calculation is also simplified as all components (axial, radial, and tangential) are expected to have same values.

In TRANSURANUS, there are currently two correlations focused on the Zircaloy cladding, i.e., the LWR and MATPRO correlations. The MATPRO correlation calculates the individual strain components separately, while the LWR correlation expects the strain to be the same in all directions (cf. Figure 1). It has to be noted that the impact of the phase transition on the thermal strain is also not modelled.

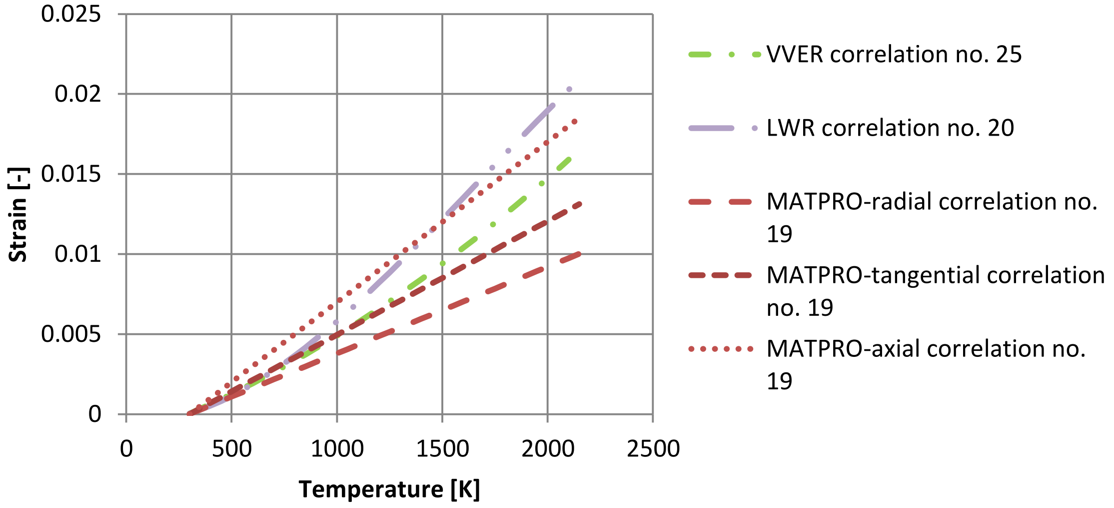

Figure 1 Thermal strain as a function of temperature for LWR and VVER conditions and from MATPRO (i.e., TRANSURANUS correlations no. 19, 20, and 25) (JRC-ITU 2014)

The FRAPCON/FRAPTRAN code additionally contains thermal strain model for Zry-4 (Luscher et al. 2011), which appears to predict experimental data rather well. This correlation is divided into two areas representing the alpha and beta phase, respectively. The transition domain can then be interpolated in-between.

The open literature research has revealed that some data on M5 thermal strain behaviour are also available, specifically in the non-proprietary version of the COGEMA (AREVA NC) technical report (Mitchel et al. 2000). These data show the thermal strain for both radial and axial directions, cf. Figure 2. Dilatometric behaviour of a Zr-base alloy having hexagonal lattice symmetry, and specifically the effect of the α to β phase transition, has also been reported in (Brachet et al. 1998).

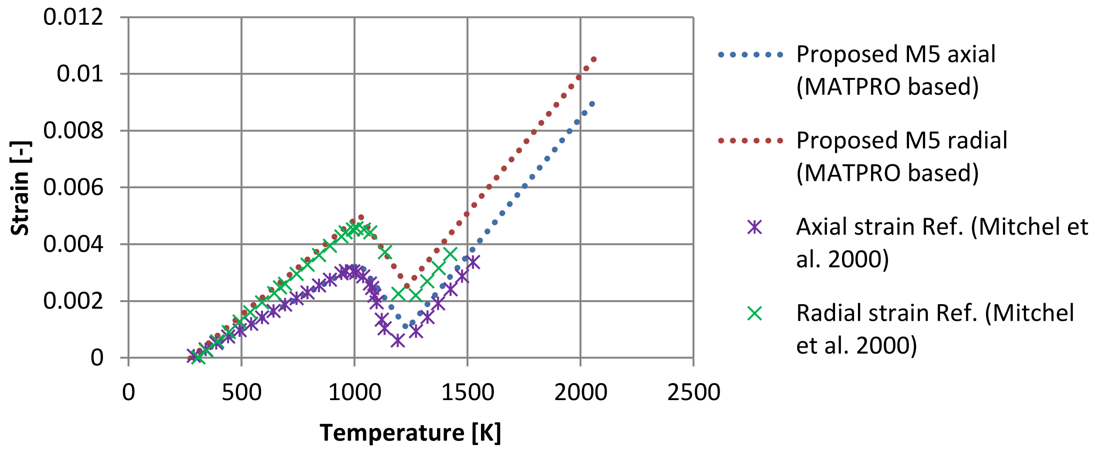

Figure 2 Thermal strain of M5 as a function of temperature. The proposed M5 correlation is also displayed (Mitchel et al. 2000), (Luscher et al. 2011)

Using the agreed M5 phase equilibrium transition temperatures ($t_{\alpha > \alpha+\beta}$ = 1023.15 K and $t_{\alpha+\beta > \beta}$ = 1233.15 K, cf. also sub-section 3.8)[3], the FRAPCON/FRAPTRAN correlation

[3] The temperatures of the phase transition measured during the thermal strain experiment of which values are given in (Mitchel et al. 2000) and which served as a basis to develop the proposed M5 correlation are about 60 K too low. This fact was also recognised in (FRAMATOME 2002). The proposed M5 thermal strain correlation takes this fact into account by assuming the correspondingly later onset and end of the phase transition.

originally developed for Zry-4 was fitted to the M5 data from (Mitchel et al. 2000), cf. Figure 2. The phase transition range was interpolated between the ranges corresponding to alpha and beta phases. The correlation is described in Eqs. 1 through 6. The ambient temperature (293.15 K) was chosen as the reference temperature point.

T < 1023.15 K

$$\varepsilon_{axial} = -2.506 * 10^{-5} + 4.441 * 10^{-6} * (T - 273.15) \quad (1)$$
$$\varepsilon_{radial} = -2.373 * 10^{-5} + 6.721 * 10^{-6} * (T - 273.15) \quad (2)$$

1023.15 K ≤ T ≤ 1233.15 K (interpolation)

$$\varepsilon_{axial} = 0.01150 - 1.092 * 10^{-5} * (T - 273.15) \quad (3)$$
$$\varepsilon_{radial} = 0.01396 - 1.193 * 10^{-5} * (T - 273.15) \quad (4)$$

T > 1233.15 K

$$\varepsilon_{axial} = -8.3 * 10^{-3} + 9.7 * 10^{-6} * (T - 273.15) \quad (5)$$
$$\varepsilon_{radial} = -6.8 * 10^{-3} + 9.7 * 10^{-6} * (T - 273.15) \quad (6)$$

where temperature T is in K and the thermal strain components ε are dimensionless.

3.5.2 Conclusion

As it might be observed in Figure 1 and Figure 2, the LWR, VVER and the proposed M5 correlations provide very similar estimates of the thermal strains at the low temperature range up to the onset of the respective phase transitions (~1000 K). At higher temperatures, the predicted thermal strain values vary substantially, as the original TRANSURANUS correlations do not take the phase transition in account.

Based on the available experimental data (Mitchel et al. 2000), the proposed M5 correlation allows an explicit prediction of axial and radial strains, taking the phase transition into account. In absence of any experimental data, the tangential strain is proposed to be calculated the same as the radial thermal strain similarly to approach adopted by the original TRANSURANUS correlations (no. 20 and 25)[4]. Consequently, the future development activities on M5 should be focused on the determination of the tangential component of M5.

3.5.3 Draft Correlation – THSTRN

```
 221   continue

!      M5 alloy
!      ==========
!      tc is temperature in Celsius
!      ====================
       if (tc .lt. 750.) then
!      ====================

       etax = -2.506e-05 + 4.441e-06 * tc
       etad = -2.373e-05 + 6.721e-06 * tc
!        ++++
!    ==============================
     else if (tc .lt. 960. ) then
!    ==============================

         etax = 0.01150 - 1.092e-05 * tc
         etad = 0.01396 - 1.193e-05 * tc
!        ++++
!    ==============================
     else
```

[4] For which thermal strain is expected to be the same for all components.

```
!    ==============================

       etax =  -8.3e-03 + 9.7e-06 * tc
       etad =  -6.8e-03 +9.7e-06 * tc
!      ======
     end if
!      ======
      eta (igrob,i,1,6) = etad
      eta (igrob,i,2,6) = etad
      eta (igrob,i,3,6) = etax
     goto 2500
!      ++++++
```

3.6 Thermal Conductivity

The thermal conductivity of the cladding is calculated in the subroutine LAMBDA. The current version of the TRANSURANUS code includes the correlations for Zircaloy[5] and E110 (JRC-ITU 2014).

3.6.1 Analysis

Brief summary of all currently implemented correlations is provided in Table 5. A comparison is given in Figure 3.

Table 5 TRANSURANUS correlations for the thermal conductivity of zirconium based cladding (JRC-ITU 2014)

Correlation	Basic description
19	Zircaloy thermal conductivity based on the MATPRO handbook
20	Standard LWR, identical to no. 19
22	Lassmann & Moreno Zircaloy correlation[6]
25	Zr1Nb VVER cladding material

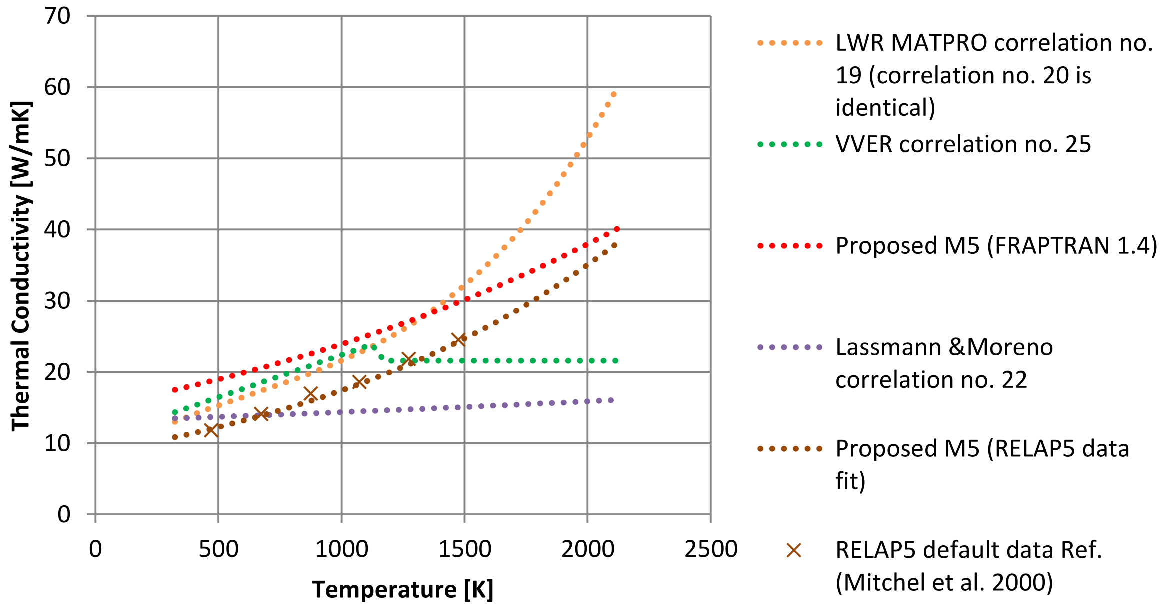

Figure 3 Thermal conductivity as a function of temperature (existing correlations in TRANSURANUS and the proposed correlations for M5) (JRC-ITU 2014), (Mitchel et al. 2000), (Luscher et al. 2011)

5 There is in general little information available about the Zircaloy cladding materials used in experiments. Therefore, TRANSURANUS sometimes does not distinguish between Zry-2 and Zry-4, even though there might be non-negligible differences.

6 The correlation will be removed in future releases of the code.

FRAPCON (Luscher et al. 2011) recommends the use of default conductivity for Zircaloy, which is deemed to be applicable to Zircaloy-2, Zircaloy-4, ZIRLO, as well as M5. This correlation is identical to the already implemented LWR MATPRO correlations no. 19 & 20.

The FRAPTRAN 1.4 code also includes the correlation of the ZrNb1 alloy, which is described by Eqs. 7 and 8 as also displayed in Figure 3.

$$\lambda = 15.0636 * e^{(0.000461843*T)} \qquad T \leq 2133\ \text{K} \tag{7}$$

$$\lambda = 36 \qquad T > 2133\ \text{K} \tag{8}$$

where temperature T is in K and thermal conductivity λ in W/m·K.

Additionally, the NRC-approved AREVA report (Mitchel et al. 2000) considers the RELAP5 (default) data as being adequate to represent the thermal conductivity of the M5 alloy. A correlation based on the interpolation of these data is given in Eq. 9.

$$\lambda = 8.6383 * e^{(0.0007*T)} \qquad T \leq 2133\ \text{K} \tag{9}$$

where temperature T is in K and thermal conductivity λ in W/m·K.

3.6.2 Conclusion

Based on information provided in (Mitchel et al. 2000) and comparison of models displayed in Figure 3 it can be deduced that correlations corresponding to LWR and VVER conditions (no. 19 and 25) and the proposed M5 follow same trend and yield similar results at low temperature range (until the onset of the phase transition). At higher temperatures the thermal conductivity values vary significantly.

Giving the above and following the assessments of data in Figure 3, this study therefore proposes to adopt the FRAPTRAN based correlation (providing slightly higher thermal conductivity values) as default thermal conductivity to be used for M5 in TRANSURANUS. The RELAP5 based correlation might also be implemented in future to provide user the flexibility of choice.

3.6.3 Draft Correlation – LAMBDA

FRAPTRAN version (default)

```
226   continue
!      M5 alloy correlation from the MATPRO handbook
!      =================
       If (tk .gt. 2133.) Then
!      =================
       lambd0 = 36.
!      =================
       Else
!      =================
       lambd0 = 15.0636*exp(0.000461843*tk)
!      =================
       EndIf
!      =================
!      --- Conversion from W/(m*K) to W/(mm*K); Statistics
       lambda = lambd0 * 0.001 * Random_Var(6,4,4)

       return
!      ++++++
```

RELAP5 based version (possibly optional)

```
227  continue
!     M5 alloy data based on the RELAP5 system code

!    =================
      lambd0 = 8.6383*exp(0.0007*tk)
!    =================

!     --- Conversion from W/(m*K) to W/(mm*K); Statistics

      lambda = lambd0 * 0.001 * Random_Var(6,4,4)

      return
!     ++++++
```

3.7 Oxide Layer Thermal Conductivity

Thermal conductivity of the oxide layer is incorporated in the OUTCOR subroutine, where each corrosion correlation uses its own value of thermal conductivity. This value can only be chosen through the corrosion model, i.e. the user cannot decide, which correlation for oxide layer thermal conductivity will be used.

3.7.1 Analysis

TRANSURANUS assumes constant values of the thermal conductivity of the zirconium oxide layer irrespective of temperature (JRC-ITU 2014). These values vary between 1.6 W/mK and 2 W/mK. The correlations are displayed in Figure 4.

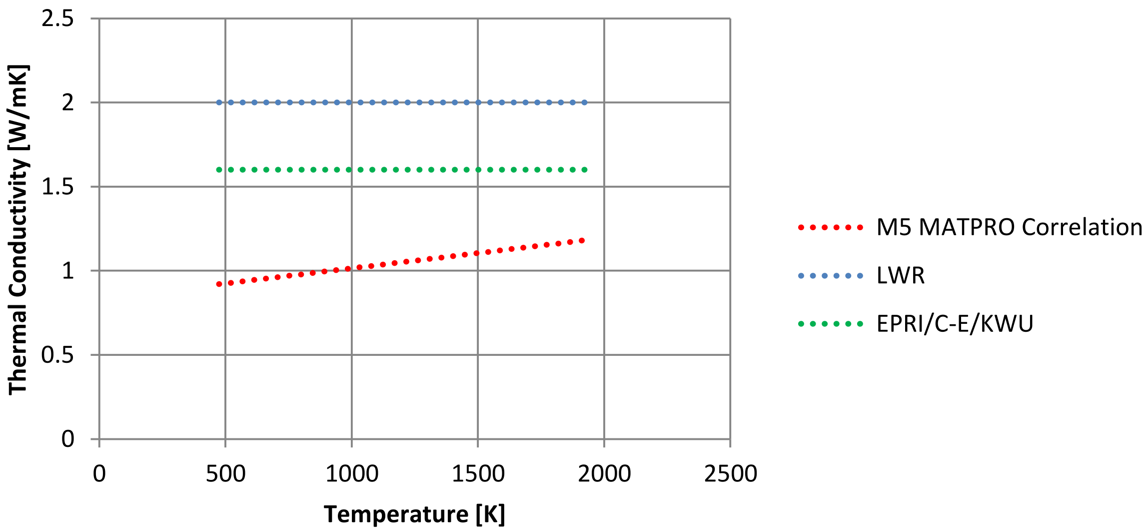

Figure 4 Comparison of the proposed and existing oxide layer thermal conductivity correlations in TRANSURANUS (JRC-ITU 2014), (Luscher et al. 2011)

The open literature research brought suitable data for M5. MATPRO correlation (Luscher et al. 2011) seems to be a good candidate due to its wide range and also conservative lower value (i.e., providing higher temperatures in oxide layer) compared to the values currently used in TRANSURANUS. The correlation is given in Eq. 10 and also displayed in Figure 4.

$$\lambda_{MATPRO} = 0.835 + 1.8 * 10^{-4} * T \qquad (10)$$

where temperature T is in K and thermal conductivity λ in W/mK.

3.7.2 Conclusion

Correlations currently implemented in TRANSURANUS provide a higher estimate of the thermal conductivity than the proposed M5 MATPRO-based correlation. In addition the proposed M5 correlation takes in account the increase of thermal conductivity with raising temperature. Draft correlation is presented in subsection 5.3.

3.8 Crystallographic Phase Transition

Crystallographic phase transition of cladding alloys is accomplished in the TRANSURANUS code by the subroutine ZRBETA. Two correlations are currently implemented in the code, representative to Zry-4 (no. 18) and E110 (no. 28) (JRC-ITU 2014).

3.8.1 Analysis

The correlation representative for Zry-4 allows the calculation of the beta phase fraction in equilibrium state and also during dynamic phases, when fast cooling or heating occurs. Beta phase fractions for both nominal and accidental-like conditions are given in Figure 5. The correlation representative for E110 allows predicting the phase transition in the equilibrium state. A comparison is given in Figure 6.

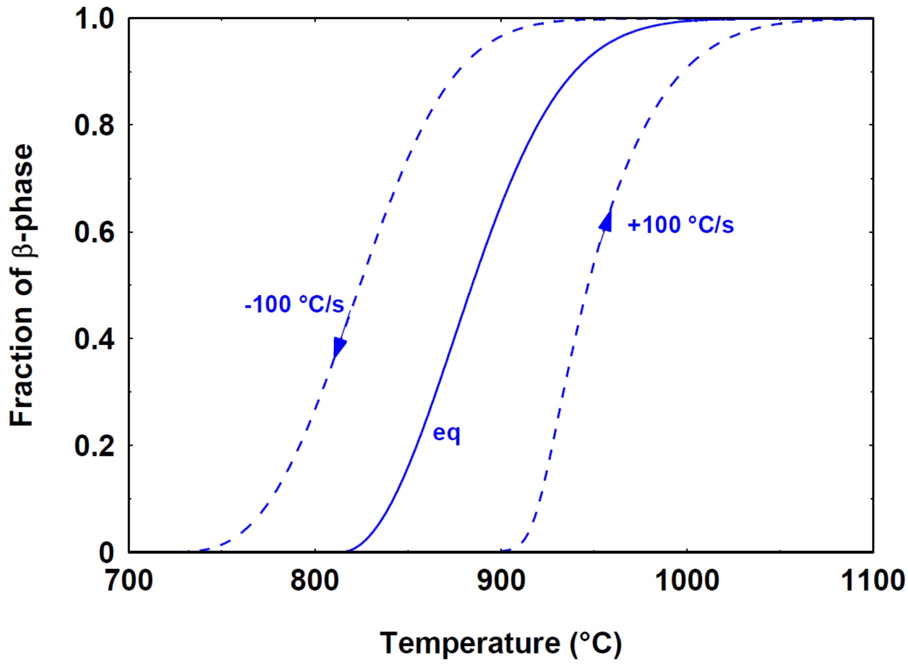

Figure 5 Zircaloy-4 β phase fraction model for nominal and accidental like conditions. The figure is adopted from (JRC-ITU 2014)

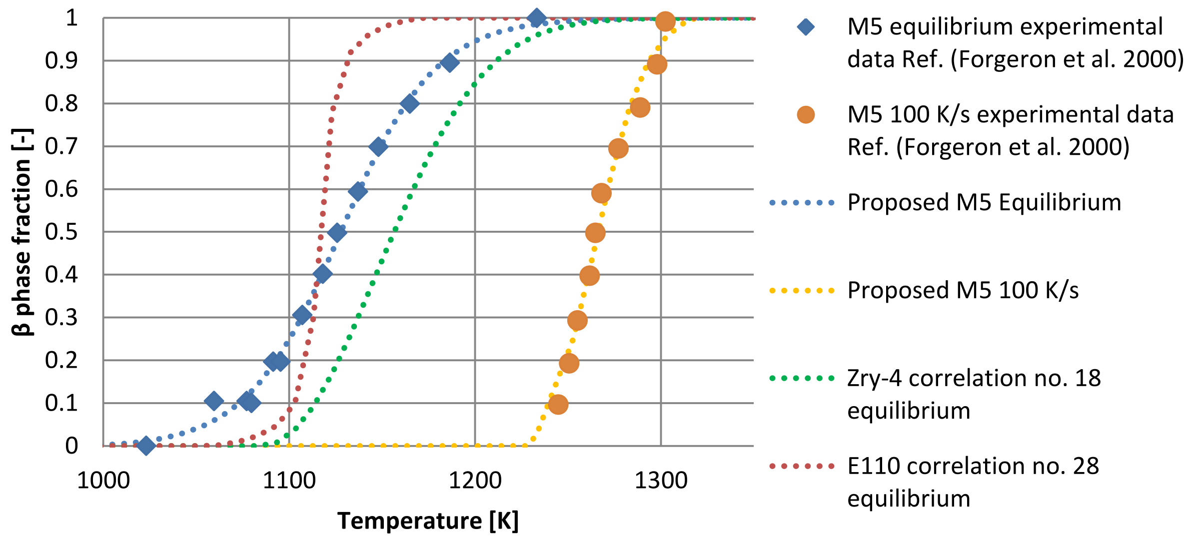

Figure 6 β phase fraction - comparison of the original TRANSURANUS correlations and the proposed M5 correlation (JRC-ITU 2014), (Forgeron et al. 2000)

Figure 6 also shows experimental data for M5 from Reference (Forgeron et al. 2000) including the exponential fit for equilibrium and accidental heat rate of 100 K/s. The proposed correlations are given in Eq. 11, which constants are given in Table 6:

$$y = a_2 + \frac{a_1 - a_2}{1 + e^{\frac{x - x_0}{dx}}} \qquad (11)$$

where:

Table 6 Phase transition correlation fit coefficients for M5

Transition type	a_1	a_2	x_0	dx
Equilibrium	-0.0048	1.00051	854.583	25.28896
100 K/s	-0.0723	1.02217	991.8829	13.7447

3.8.2 Conclusion

The proposed M5 correlation considers equilibrium and accidental-like heating rates. Further improvements are necessary to also consider the representative cooling rates (measurement data are available only for cooling rates of 8 K/min (Forgeron et al. 2000)). A sensitivity study could be performed to evaluate whether the proposed exponential fit is necessary. Note also that the effect of hydrogen on a crystallographic phase transition has shown to be non-negligible (Brachet et al. 2002), and hence shall be incorporated in future releases of TRANSURANUS as well.

3.8.3 Draft Correlation – ZRBETA

```
 221 continue

! Model for M5 alloy
! =================
!      iso : switch for dynamic model (iso=1)
! Static approach assuming thermal equilibrium:
! -------------------------------------------
!....temperatures given in degree C
    tca = 750.
    tcb = 960.
    tcad = 955.
    tcbd = 1040.
```

```
   eqa1 = -0.0048
   eqa2 = 1.00051
   eqx0 = 854.583
   eqdx = 25.28896
   dya1 = -0.0723
   dya2 = 1.02217
   dyx0 = 991.8829
   dydx = 13.7447

!  Thermal equilibrium

!    ===================
   if (iso .eq. 1) then
!    ===================
!      ++++++++++++++++++++
      if (tc .le. tca) then
!      ++++++++++++++++++++
        y = 0.0
!      ++++
      Else if (tc .le. tcb) then
!      ++++
        y = eqa2+(eqa1-eqa2)/(1+exp((tc-eqx0)/eqdx))
!      +++++++++++++++++
       Else
!      +++++++++++++++++
        y = 1.
!      ++++++
      end if
!      ++++++
!    ========================
   else if (iso .eq. 2) then
!    ========================

! Dynamic approach:

!      ++++++++++++++++++++
      if (tc .le. tcad) then
!      ++++++++++++++++++++
        y = 0.0
!      ++++
      Else if (tc .le. tcbd) then
!      ++++
        y = dya2+(dya1-dya2)/(1+exp((tc-dyx0)/ dydx))
!      +++++++++++++++++
       Else
!      +++++++++++++++++
        y = 1.
!      ++++++
      end if
!      ++++++
!    ======
   end if
!    ======

      zrbeta = y

   return
!    ++++++
```

3.9 Specific Heat at Constant Pressure

Specific heat at constant pressure is given by the correlation CP. The TRANSURANUS code currently considers two correlations, where the first is aimed at LWR conditions (no. 20) and the second at VVER conditions (no. 25) (JRC-ITU 2014).

3.9.1 Analysis

The existing correlations for the calculation of specific heat at constant pressure are shown in Figure 7.

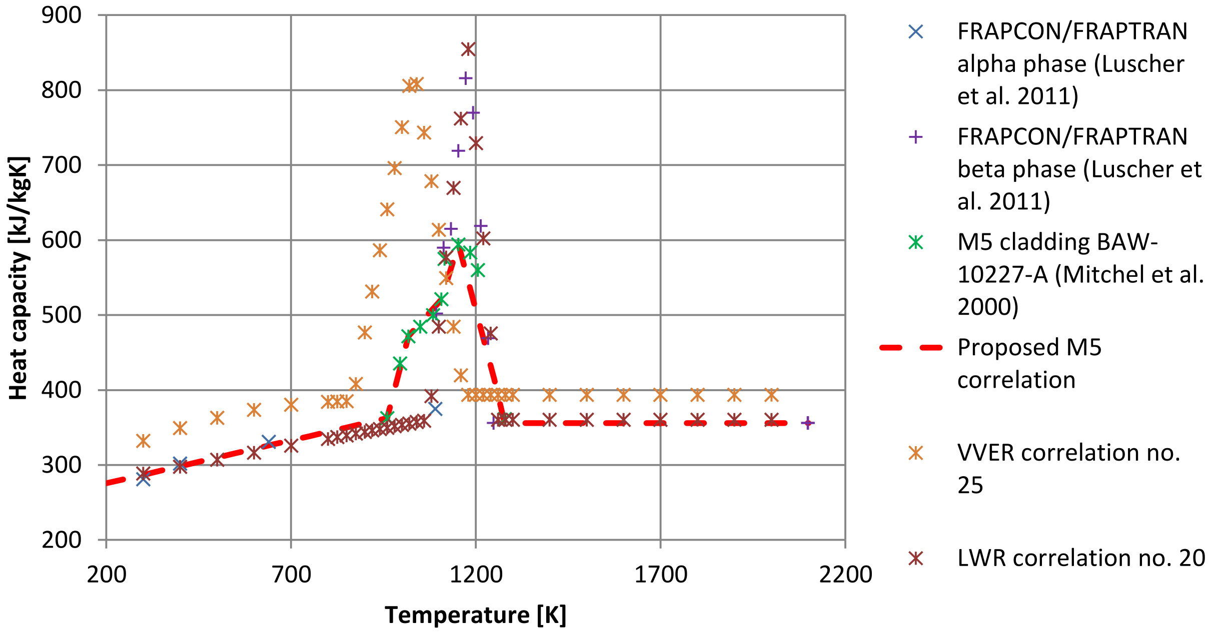

Figure 7 Heat capacity as a function of temperature (JRC-ITU 2014), (Mitchel et al. 2000), (Luscher et al. 2011)

As regards the development of a representative correlation for M5 based on the available experimental data from (Mitchel et al. 2000) and (Luscher et al. 2011) it was decided to split the problem into three parts: (i) low temperature; (ii) phase transition; and (iii) high temperature regions.

The behaviour in low and high temperature domain is based on the FRAPCON/FRAPTRAN data (Luscher et al. 2011), which were originally developed for Zircaloy-2 and are also applicable to M5. The phase transition part cannot be deduced from the FRAPCON/FRAPTRAN data due to the different behaviour of the M5 alloy. Thus, data used for the proposed M5 correlation in the phase transition domain were obtained from (Mitchel et al. 2000).

The proposed correlation for specific heat of M5 at constant pressure is given in Eqs. (12)-(17) and Figure 7.

$c_p = 0.1147 * T + 252.55$	$T < 960.122$ K	(12)
$= 1.9014 * T - 1463.1$	$960.122\ K \le T < 1017.6$ K	(13)
$= 0.5527 * T - 90.68$	$1017.6\ K \le T < 1107.8$ K	(14)
$= 1.5837 * T - 1232$	$1107.8\ K \le T < 1153.1$ K	(15)
$= -1.8617 * T + 2740.9$	$1153.1\ K \le T < 1278.2$ K	(16)
$= 356$	$T \ge 1278.2$ K	(17)

3.9.2 Conclusion

Figure 7 shows a large similarity of all correlations for specific heat in the range of low and high temperatures. In the domain of phase transition, values vary for each alloy due to the different phase transition temperatures. The proposed M5 correlation takes also this effect into account to provide representative results. Nevertheless, the large difference between the peak value of M5 in comparison with those for the other Zircaloy-based cladding materials requires further (experimental) investigation.

3.9.3 Draft Correlation – CP

```
222 continue

!    M5 alloy cladding
!    ==============
!    ========================
     if (tk .lt. 960.122) then
!    ========================
      cp0 = 0.1147*tk +252.55
!    ==============================
     else if (tk .lt. 1017.6 ) then
!    ==============================
      cp0 = 1.9014*tk  - 1463.1
!    ==============================
     else if (tk .lt. 1107.08 ) then
!    ==============================
      cp0 = 0.5527*tk  - 90.68
!    ==============================
     else if (tk .lt. 1153.1 ) then
!    ==============================
      cp0 = 1.5837*tk  - 1232.
!    ==============================
     else if (tk .lt. 1278.2 ) then
!    ==============================
      cp0 = -1.8617*tk  + 2740.9
!    ==============================
     else
!    ==============================
      cp0 = 356.
!    ======
     end if
!    ======
!      --- Conversion from J / (kg*K) to J / (g*K), statistics
     cp  = cp0 * 1.e-03 * Random_Var (13,4,4)
     return
!    ++++++
```

4. Mechanical properties

4.1 Poisson's Ratio

Poisson’s ratio is given by the subroutine NUELOC. The TRANSURANUS code has implemented data for LWR and VVER cladding materials, correlations no. 20 and 25, respectively.

4.1.1 Analysis

Poisson’s ratios are displayed as a function of temperature in Figure 8. While the VVER correlation is a linearly decreasing function of temperature, the LWR correlation is constant and equal to 0.32. For temperatures above the melting point (2128.15 K), a residual value of 0.05 is chosen in the latter.

For M5, according to the COGEMA (AREVA NC) technical report (accepted by US NRC) (Mitchel et al. 2000), Poisson’s ratio for M5 should be set to 0.37 irrespective of temperature.

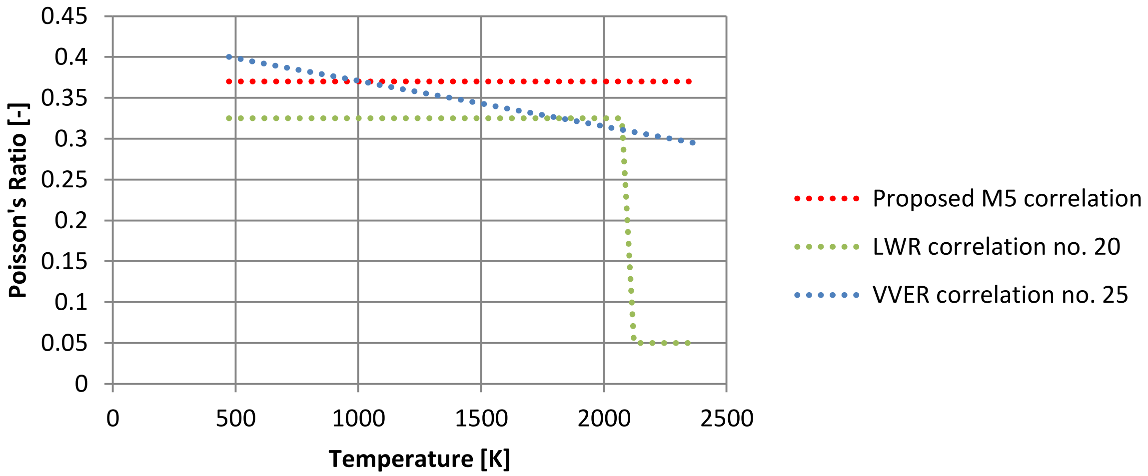

Figure 8 Poisson's ratio as a function of temperature for LWR, VVER (E110), and M5 (JRC-ITU 2014), (Mitchel et al. 2000)

4.1.2 Conclusion

All the already implemented correlations give values typical to steels.

Following the recommendation of COGEMA’s technical report (Mitchel et al. 2000), it is proposed to choose Poisson’s ratio of M5 as equal to 0.37, independent of material temperature.

Experimental data on M5 behaviour would again be necessary to propose possibly more accurate correlation for Poisson’s ratio of M5.

4.1.3 Draft Correlation – NUELOC

```
 221   continue

!     M5 alloy
!     =========
!     Typical value adopted by AREVA for M5

      nueloc = 0.37 * Random_Var(3,4,4)

      return
!     ++++++
```

4.2 Elasticity Constant

Young's Modulus (E) is calculated in TRANSURANUS by the ELOC subroutine. In the code, the correlations applicable to LWR type claddings include LWR correlation (no. 20) and VVER correlation (no. 25).

4.2.1 Analysis

In the open literature sources, the topic is treated specifically by (Mitchel et al. 2000), which recommends using the RELAP5 correlation for M5. This correlation has originally been developed for Zircaloy-4, but it is deemed to provide appropriate results also for M5.

The RELAP5 correlation is divided into four temperature intervals and listed below in Eqs. (18) through (21).

$$E = 1.088 * 10^5 - 5.475 * 10^1 * T \qquad T \leq 1090\ \text{K} \tag{18}$$

$$= 1.017 * 10^5 - 4.827 * 10^1 * T \qquad 1090\ \text{K} < T \leq 1240\ \text{K} \tag{19}$$

$$= 9.210 * 10^4 - 4.050 * 10^1 * T \qquad 1240\ \text{K} < T \leq 2027\ \text{K} \tag{20}$$

$$= 1.0 * 10^4 \qquad 2027\ \text{K} < T \tag{21}$$

where temperature T is in K and Young's Modulus E in MPa.

A comparison of the RELAP5 correlation with correlations implemented in the TRANSURANUS code for LWR and VVER claddings is given in Figure 9.

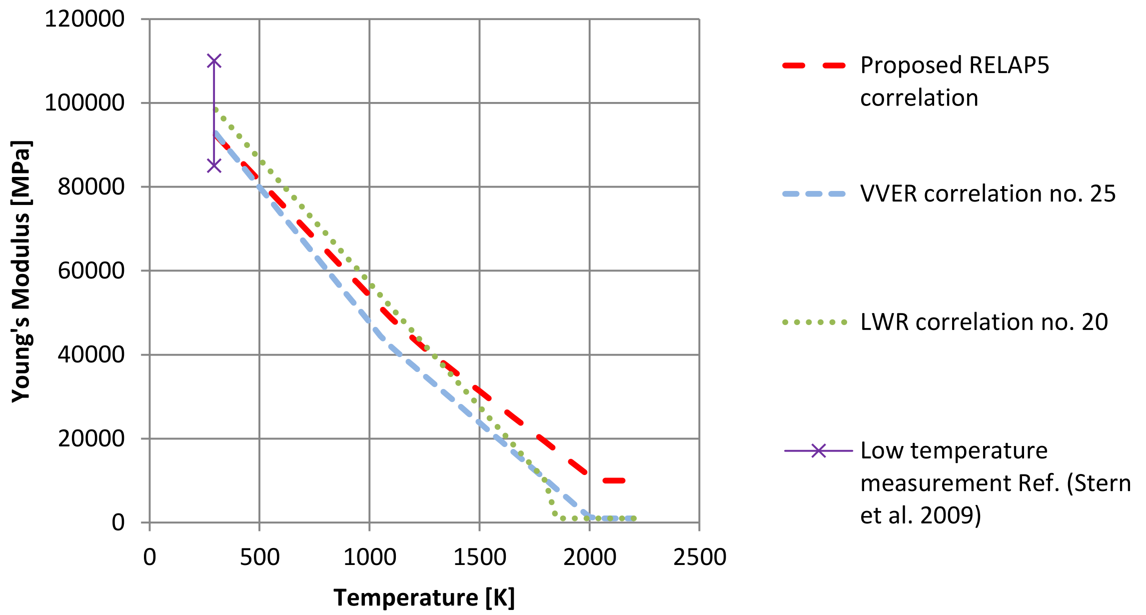

Figure 9 Young's Modulus as a function of temperature (the RELAP5 correlation for Zircaloy-4 recommended for M5 compared to the TRANSURANUS correlations for LWR conditions and VVER conditions (E110)) (JRC-ITU 2014), (Mitchel et al. 2000), (Stern et al. 2009)

As can be observed, the RELAP5 correlation provides values similar to those provided by the LWR and VVER correlations for temperatures up to about 1600 K. The RELAP5 correlation further retains a non-negligible value of Young's Modulus at higher temperatures (representative to accidental conditions) allowing the material to retain a certain degree of residual stiffness up to the melting point. This is consistent with the dynamic modulus measurements indicating that the true modulus does not approach zero as the melting point is reached (Hayden et al. 1965).

Young's Modulus given by the RELAP5 correlation is also consistent with the one value measured for M5 at room temperature and available in the open literature (Stern et al. 2009).

4.2.2 Conclusion

Given the above, the RELAP5 correlation is proposed to be implemented in the TRANSURANUS code as representative for M5 alloy. Experimental data on M5 behaviour, including high-temperature and any possible irradiation effects, would be necessary to propose possibly more accurate correlation for Young's Modulus of M5. During loss-of-coolant accident (LOCA) conditions, however, the change of elastic modulus is notably smaller than that of the thermal strain. Hence, in these circumstances, further refinement of Young's modulus seems to be of secondary importance.

4.2.3 Draft Correlation – ELOC

```
 221   continue

!     ==========
!     M5 alloy
!    ===========
!     ====================
      if (tk .le. 1090.) then
!     ====================

        esolid =1.088e5 - 5.475e1 * tk
!    ==============================
     else if (tk .le. 1240. ) then
!    ==============================

        esolid =1.017e5- 4.827e1*tk
!    ==============================
     else if (tk .le. 2027. ) then
!    ==============================

        esolid =9.210e4 - 4.050e1*tk
!    ==============================
     else
!    ==============================

        esolid = 1.e4
!     ======
      end if
!     ======
       eloc   = esolid * Random_Var(2,4,4)
!     =========================
      if (eloc.lt.eminh) eloc = eminh
!     =========================

      return
!     ++++++
```

4.3 Yield Stress

Another important mechanical characteristic is the yield stress, which is calculated in the TRANSURANUS subroutine SIGSS. The TRANSURANUS code currently includes yield stress correlations for LWR (no. 20) and VVER (no. 25) type claddings (JRC-ITU 2014).

4.3.1 Analysis

While the correlation corresponding to VVER conditions provides yield stress values as a function of temperature, the correlation corresponding to LWR conditions[7] gives a constant value of 350 MPa in the entire temperature range considered, cf. Figure 10. This initial value seems to be an oversimplification, and needs to be modified in view of information in the open literature.

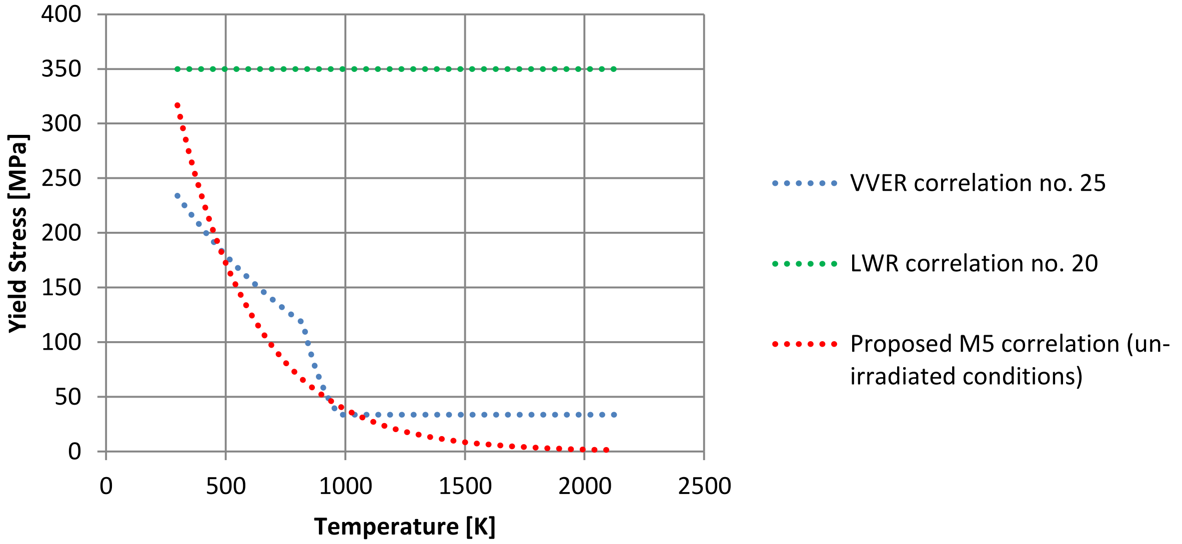

Figure 10 Yield stress correlations for un-irradiated fuel claddings corresponding to (JRC-ITU 2014), (Stern et al. 2009), (Cazalis et al. 2005)[8]

Open literature provides data on yield stress temperature dependency for both irradiated and non-irradiated M5 material samples (Stern et al. 2009), (Cazalis et al. 2005), cf. Figure 11.

For the un-irradiated material two functional dependencies could be reconstructed, which describe yield stress of M5 in longitudinal and transversal directions, respectively (Stern et al. 2009). Conservatively, the longitudinal (LD) dependency is proposed to be chosen as a reference M5 yield stress correlation in the un-irradiated conditions.

(Cazalis et al. 2005) provides two sets of data for irradiated material. The first corresponds to 5 cycle (approx. 57 – 64 GWd/tU) irradiation, the second one to 6 cycle (approx. 75 GWd/tU) irradiation conditions. It has to be noted that for the high burnup the measured yield stress of M5 is consistently lower than for the lower burnup samples. Not enough information is available in the report on the exact conditions of the irradiation, neither on the measurement uncertainties, but considering the typical influence of the radiation hardening on yield stress, an opposite effect would be expected.

Following again a conservative approach, the functional dependency for higher burnup (with lower measured values of the yield stress) was chosen as the upper reference dependency corresponding to the irradiated conditions.

[7] The range of material validity is not specified in the TRANSURANUS handbook.

[8] The correlation no. 25 probably shows a decrease of yield stress in the temperature range between approx. 823 K to 973 K due to phase transition. However, this does not correspond to the phase transition temperatures of E110 given in TRANSURANUS (approx. 1050 K to 1173 K) (JRC-ITU 2014).

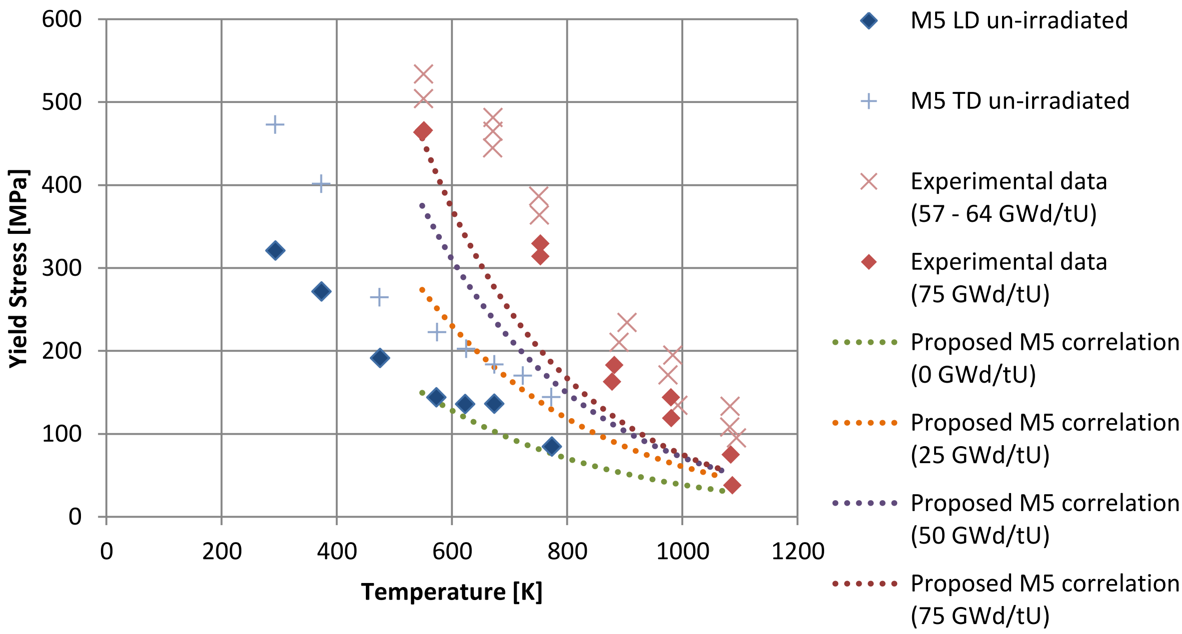

Figure 11 Yield stress as a function of temperature and burnup. LD = longitudinal & TD=transversal directions (Stern et al. 2009), (Cazalis et al. 2005)

Based on the aforesaid assumptions, a correlation describing the yield stress of M5 has been developed as a function of temperature and burnup, cf. Eq. 22:

$$\sigma_{0.02} = (13.736 * burnup + 341.33) * \mathrm{e}^{-(1.333*10^{-5}*\mathrm{burnup}+3*10^{-3})*(T-273.15)} \quad (22)$$

where the yield stress $\sigma_{0.02}$ is in MPa, temperature T in K, and burnup in GWd/tU.

4.3.2 Conclusion

The above discussion demonstrates large differences in the treatment of yield stress in TRANSURANUS. The correlation for the LWR condition seems to be over-simplified, as it does not take into account the decrease of yield stress with increasing temperature. This should be updated on the basis of available information in the open literature.

The proposed M5 and the original E110 correlation take the influence of temperature explicitly into account. They also follow the same trend.

In the field of nominal as well as accidental operating conditions, the proposed M5 correlation gives more conservative values, in the sense of providing lower estimates of the yield stress. Furthermore, the proposed correlation takes in account also the irradiation hardening of the material.

4.3.3 Draft Correlation – SIGSS

```
 221  continue
!    === M5 alloy
!    ================================
!      variable burnup must be defined under local data as     burnup = 0.001 * BRNUP1(lschni,1)

     sigss0 = (13.736*burnup+341.33)*exp(-(1.3333e-5*burnup+0.003)*tc)
     sigss = sigss0 * Random_Var (8,4,4)

     return
!    ++++++
```

4.4 Strain due to Irradiation Induced Swelling

The phenomenon of irradiation induced swelling is treated in TRANSURANUS in the subroutine SWELOC. TRANSURANUS currently includes correlations for Zircaloy-2 (Zry-2), Zry-4 and E110 alloys. Applicability to M5 is however not specified (JRC-ITU 2014). It is also to be noted that the Zircaloy growth is strongly influenced by the texture, which is often unknown.

4.4.1 Analysis

The correlations implemented in the TRANSURANUS code are listed in Table 7. Graphical comparison is given in Figure 12 through Figure 18. The strain is given in relative units and the neutron fluence is given in neutrons per square centimetre (consistently with the TRANSURANUS Handbook (JRC-ITU 2014)). While correlations 17 through 19 and 21 allow prediction of swelling only in axial direction others, namely 20, 25, and 26, include prediction of all swelling components (axial, radial, and tangential).

Table 7 TRANSURANUS correlations for strain due to irradiation induced swelling (JRC-ITU 2014)

Correlation	Basic description	Predicted strain component[9]
17	PWR, stress relieved Zry-4	Axial
18	PWR, stress relieved Zry-4	Axial
19	MATPRO-data for Zry-2 and Zry-4	Axial
20	Annealed/small cold work Zircaloy[10]	Axial, radial, tangential
21	Cold worked, stress relieved Zry-2 and Zry-4	Axial
25	VVER (E110)	Axial, radial, tangential
26	VVER (E110)	Axial, radial, tangential

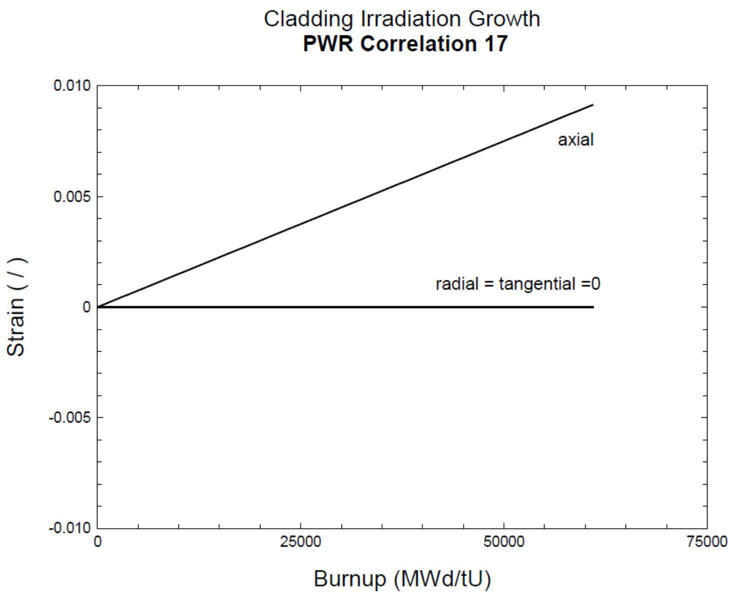

Figure 12 Strain due to irradiation induced swelling for Zry-4 - correlation 17. Figure adopted from (JRC-ITU 2014)

9 The strain models are often simplified and not taking into account all strain components.

10 There is in general little information available about the Zircaloy cladding materials used in experiments. Therefore, TRANSURANUS sometimes does not distinguish between Zry-2 and Zry-4, even though there might be non-negligible differences.

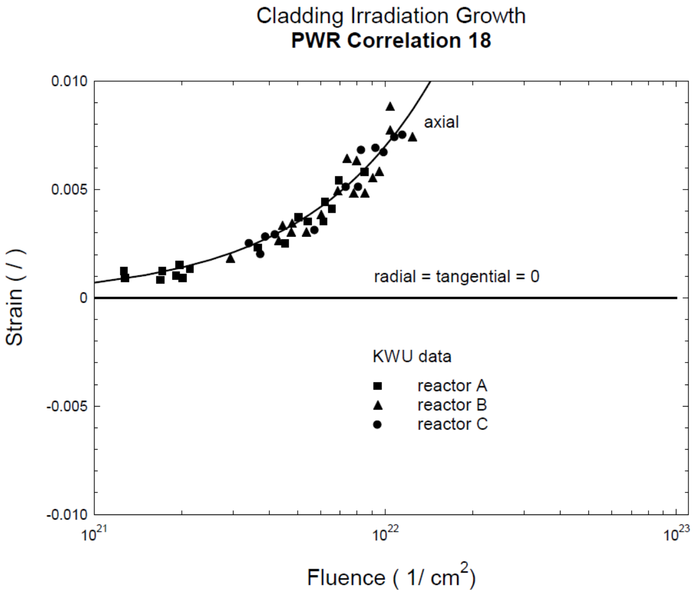

Figure 13 Strain due to irradiation induced swelling for Zry-4 - correlation 18. Figure adopted from (JRC-ITU 2014)

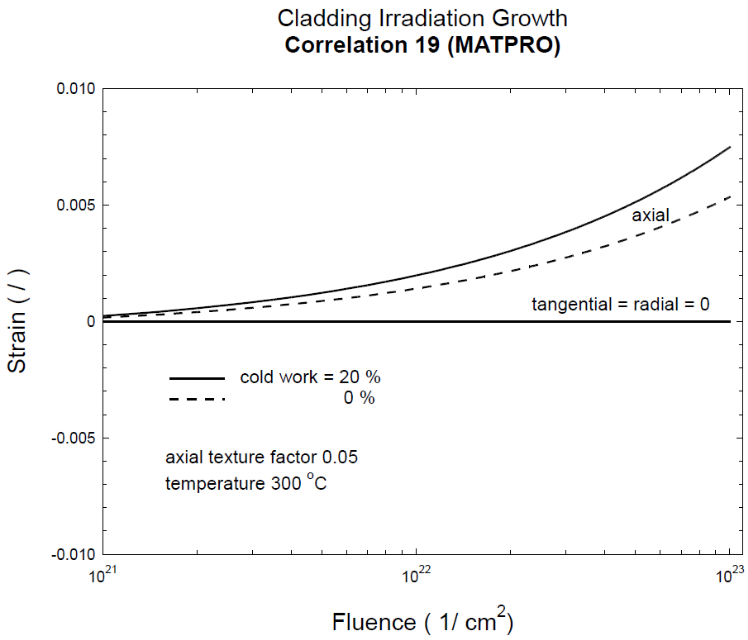

Figure 14 Strain due to irradiation induced swelling for Zry-2 & Zry-4[11] - correlation 19. Figure adopted from (JRC-ITU 2014)

11 The irradiation induced swelling is modelled the same for both alloys Zircaloy-2 & 4 (JRC-ITU 2014).

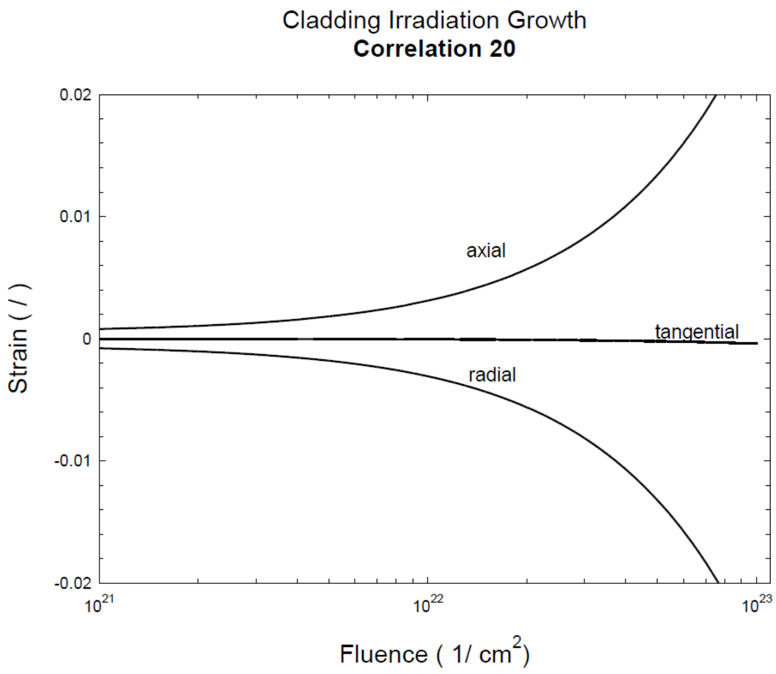

Figure 15 Strain due to irradiation induced swelling for Zircaloy[12] - correlation 20. Figure adopted from (JRC-ITU 2014)

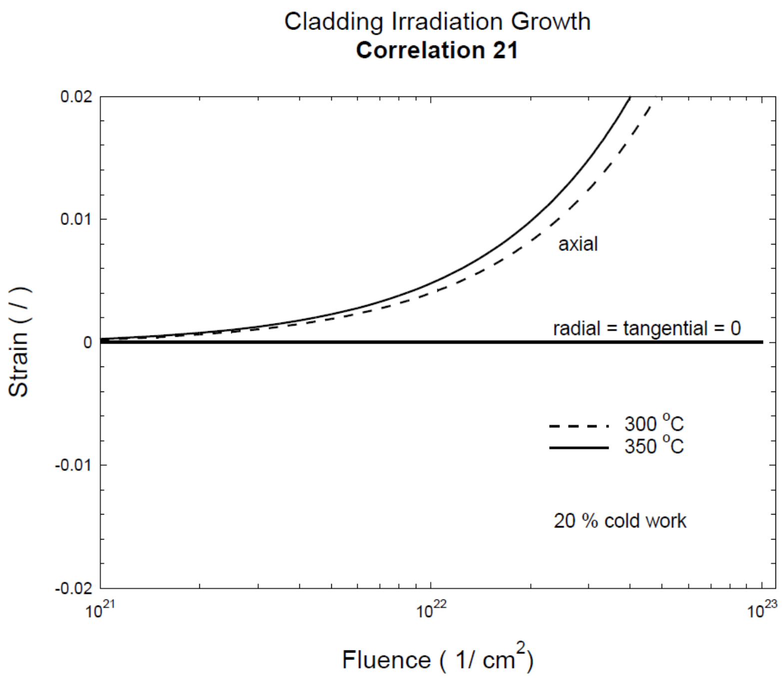

Figure 16 Strain due to irradiation induced swelling for Zry-2 & Zry-4 - correlation 21. Figure adopted from (JRC-ITU 2014)

[12] There is in general little information available about the Zircaloy cladding materials used in experiments. Therefore, TRANSURANUS sometimes does not distinguish between Zry-2 and Zry-4, even though there might be non-negligible differences.

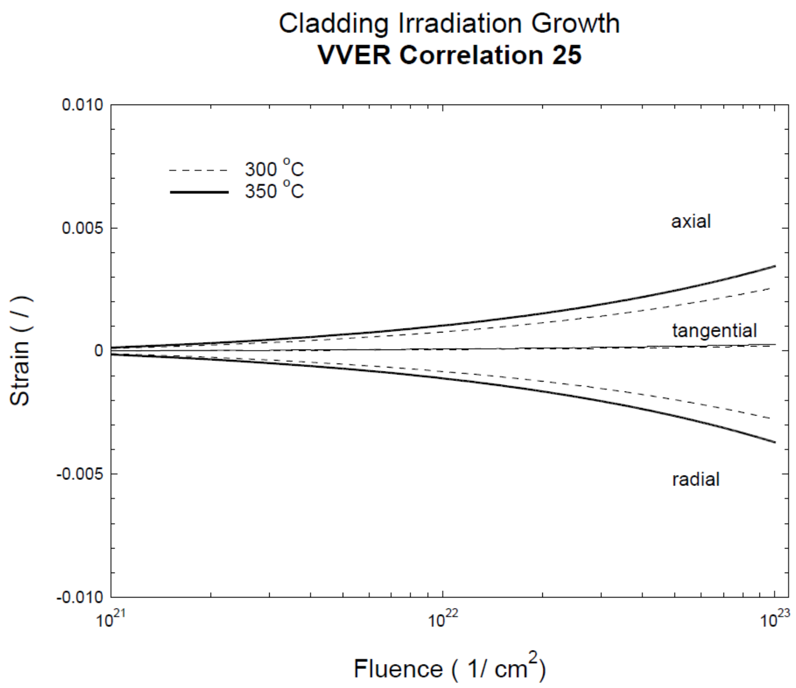

Figure 17 Strain due to irradiation induced swelling for VVER conditions (E110) - correlation 25. Figure adopted from (JRC-ITU 2014)

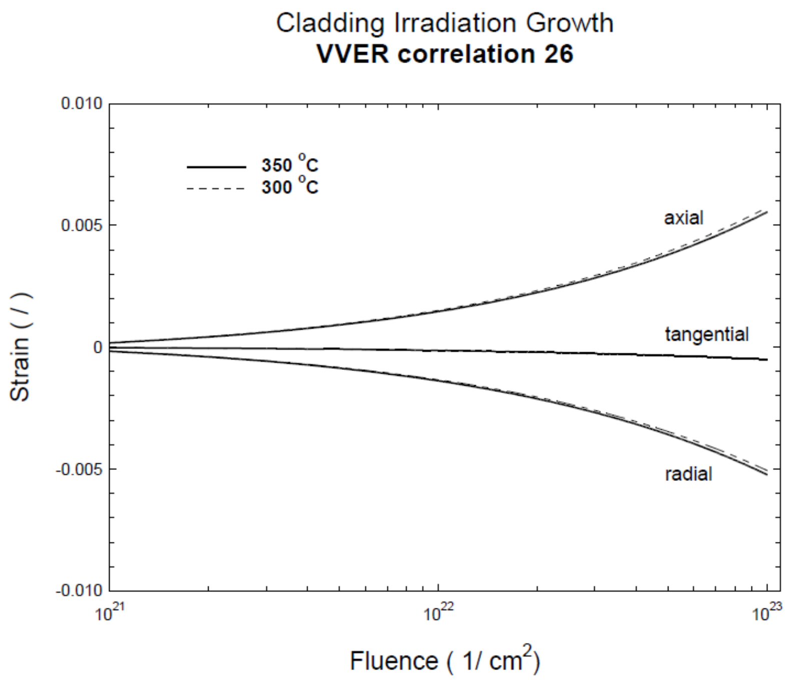

Figure 18 Strain due to irradiation induced swelling for VVER conditions (E110) - correlation 26. Figure adopted from (JRC-ITU 2014)

For M5, MATPRO recommends using the correlation given in Eq. (23) to predict its irradiation induced axial growth/swelling (Luscher et al. 2011).

$$\varepsilon_{ax.swell} = 7.013 * 10^{-21} * \varphi^{0.81787} \qquad (23)$$

where φ is fast neutron fluence (i.e., E > 1.0 MeV) in n/cm^2.

As displayed in Figure 19, the correlation seems to fit the operational data with a reasonable accuracy including the domain of high burnup. Note, however, that the MATPRO correlation allows only the prediction of axial strains.

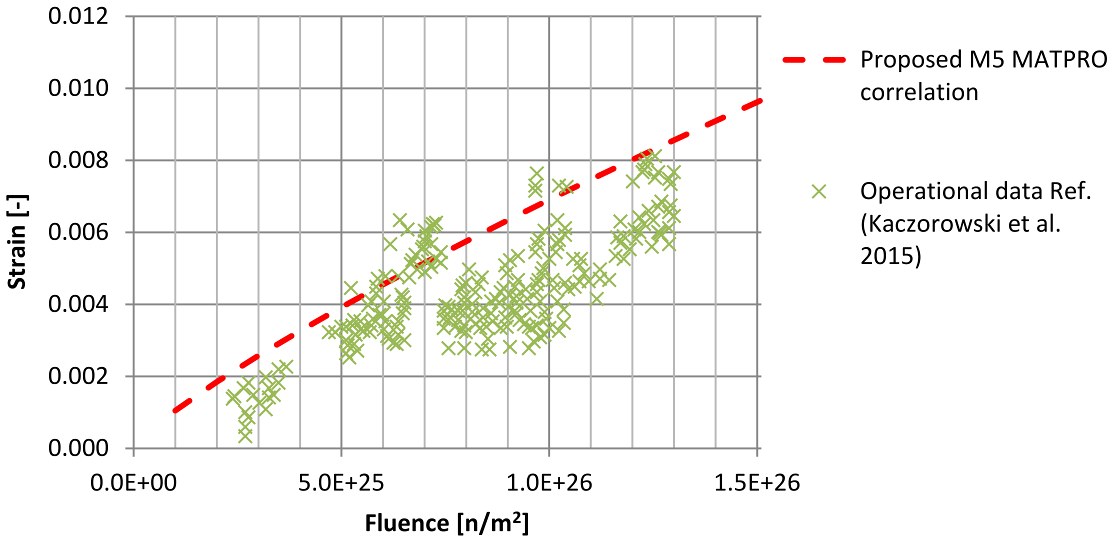

Figure 19 Axial irradiation induced growth/swelling (M5 MATPRO correlation) (Luscher et al. 2011), (Kaczorowski et al. 2015). To compare the proposed M5 correlation with operational data, it was assumed that 50 GWd/tU corresponds to neutron fluence of 10^{26} n/m^2 (Bossis et al., 2009).

4.4.2 Conclusion

Assessment of the currently implemented correlations for the cladding irradiation induced growth showed that the predicted growth values vary significantly.

As regards the behaviour of M5 it is proposed to use the MATPRO correlation (FRAMATOME 2002) as it seems to fit the available experimental data with acceptable accuracy. In accordance with the basic principle of cladding growth and the approach implemented for the existing TRANSURANUS correlations no. 20, 25 and 26, it is also proposed to assume that the change of the radial component is the same as of the axial component, but with the latter having an opposite sign in order to preserve the volume balance.

4.4.3 Draft Correlation – SWELOC

```
222  continue
!      M5 alloy MATPRO

        if (implic.eq.1) return
!                   ++++++
         flznew = fluxti(lschni,1)
         flzold = fluxti(lschni,2)
         swe1 = 7.013e-21*flzold**0.81787
         swe2 = 7.013e-21*flznew**0.81787
        deltas = swe2-swe1
       eta(igrob,i,1,7) = eta7 (igrob,i,1) -deltas*Random_Var(4,4,4)
       eta(igrob,i,2,7) = eta7 (igrob,i,2) + 0.*Random_Var(4,4,4)
       eta(igrob,i,3,7) = eta7 (igrob,i,3) + deltas*Random_Var(4,4,4)
       goto 3000
!      +++++++++
```

4.5 Creep Anisotropy Coefficients

The creep anisotropy coefficients are calculated in the TRANSURANUS subroutine ANISOTRP. Each material is characterised by three main coefficients F, G and H, out of which effective stress can be calculated according to the following equation (Eq. 24):

$$\sigma_{eff} = \sqrt{F(\sigma_r - \sigma_t)^2 + G(\sigma_t - \sigma_a)^2 + H(\sigma_a - \sigma_t)^2} \tag{24}$$

where σ_r, σ_t, σ_a are the stresses in the radial, tangential, and axial directions, respectively. The creep rate components in the three directions can then calculated using the effective creep rate ε_{eff} according to (Eq. 25):

$$\begin{aligned}
\dot{\varepsilon_r} &= \frac{\dot{\varepsilon_{eff}}}{\sigma_{eff}}[(H+F)\sigma_r - F\sigma_t - H\sigma_a] \\
\dot{\varepsilon_t} &= \frac{\dot{\varepsilon_{eff}}}{\sigma_{eff}}[(F+G)\sigma_t - G\sigma_a - F\sigma_r] \\
\dot{\varepsilon_a} &= \frac{\dot{\varepsilon_{eff}}}{\sigma_{eff}}[(G+H)\sigma_a - H\sigma_r - G\sigma_t]
\end{aligned} \tag{25}$$

Consequently, TRANSURANUS uses these values to calculate the directional strains.

For materials exhibiting isotropic behaviour F, G, and H are all equal to 0.5, while for non-isotropic materials these coefficients vary.

The TRANSURANUS code contains creep anisotropy coefficients for both Zircaloy-4 and E110.

4.5.1 Analysis

Zircaloy-4 – anisotrp18.f95, crpc18matdata.f95 (JRC-ITU 2014)

The TRANSURANUS code contains creep anisotropy coefficients for Zircaloy-4. The parameters are different for the alpha and beta phases and the transition range is interpolated between those values. It is noted that the beta phase of Zry-4 is treated like an isotropic material. All coefficients are listed in Table 8.

Table 8 Creep anisotropy coefficients for Zircaloy-4[13]

Phase	F	G	H
Alpha	0.240	0.956	0.304
Beta	0.5	0.5	0.5
Transition	coeff_alpha*(1-y) + coeff_beta*y, where y is the volume fraction of the beta phase		

Zr1Nb – VVER Correlations (JRC-ITU 2014)

At the present time, three different correlations are implemented in the TRANSURANUS code for E110. It is noted that the parameters of the correlations are constant, i.e. no influence of temperature, neutron fluence or phase transition is modelled. Coefficients for all implemented E110 correlations are listed in Table 9.

[13] It is not specified which type of Zircaloy-4 (i.e., SRA or RXA) is referred to.

Table 9 Creep anisotropy coefficients for E110

Number	Additional information	F	G	H
25	Standard version	0.18	0.62	0.38
26	New with time hardening	0.063	0.859	0.552
27	Old with time hardening	0.063	0.859	0.552

A careful reader might observe that, even though the correlations 26 and 27 are listed as time hardening versions, the coefficients are not time / fluence dependent. Furthermore, creep anisotropy coefficients are same in both correlations. Consequently, these correlations might be considered for removal from the code since they have been earlier used only for testing purposes.

Open literature does not provide any data on the anisotropy of M5, neither does the FRAPCON/FRAPTRAN (Luscher et al. 2011).

4.5.2 Conclusion

As might be seen from paragraphs above, the coefficients vary significantly, e.g., there is no consistency between Zry-4 and E110 values. In fact, this is to be expected due to different fabrication processes and resulting material textures.

The values closest to each other are those used in the correlation 25 and for the alpha phase of Zry-4. We note that very few information is available in open literature on E110 behaviour (Rogozyanov et al. 2008).

This topic requires further research and development, including a possible measurement of creep anisotropy properties (encompassing both nominal and accidental conditions) to devise a reliable recommendation for anisotropy creep coefficients of M5. Until this can be made, it is proposed to use temporarily creep anisotropy coefficients of E110 also for M5.

4.6 Creep Rate

The material creep properties are modelled in the subroutine ETACR. The TRANSURANUS code currently includes several creep correlations (JRC-ITU 2014) which are listed in Table 10. It has to be noted that correlation no. 17 is confidential and is not part of the official code release available at JRC Petten. In this code release, the correlation no. 17 is identical to correlation no. 18.

Table 10 Existing TRANSURANUS creep rate correlations (JRC-ITU 2014)

Correlation	Basic description
Crpc17	M5, Norton law, LOCA conditions
Crpc18	Zircaloy-4, Norton law, LOCA conditions
Crpc20	Zircaloy, LWR version, operational conditions
Crpc25	VVER, MATPRO-N1 based
Crpc26	VVER, New IAE with time hardening
Crpc27	VVER, Old IAE with time hardening
Crpc28	VVER, Norton law

4.6.1 Analysis

Comparison of all implemented correlations in terms of creep strain including the below proposed M5 correlation for temperature 653.15 K and pressure 90 MPa is given in Figure 20 and Figure 21.

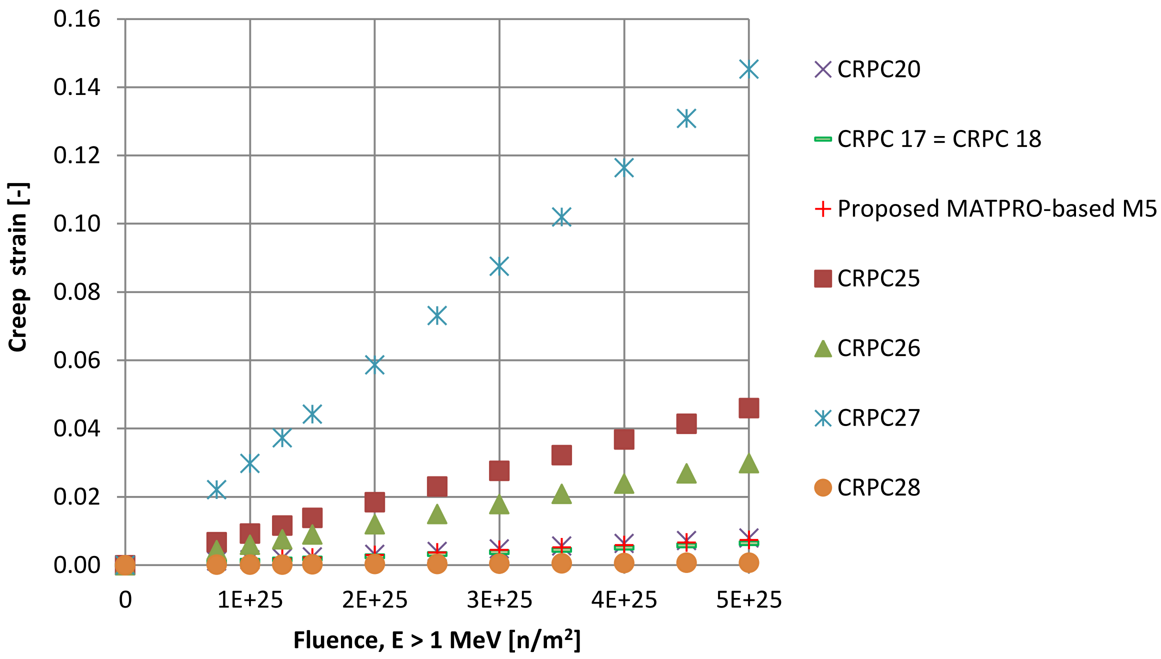

Figure 20 Comparison of creep correlations at 653.15 K and 90 MPa, (JRC-ITU 2014), (Luscher et al. 2011), (Gilbon et al. 2000)

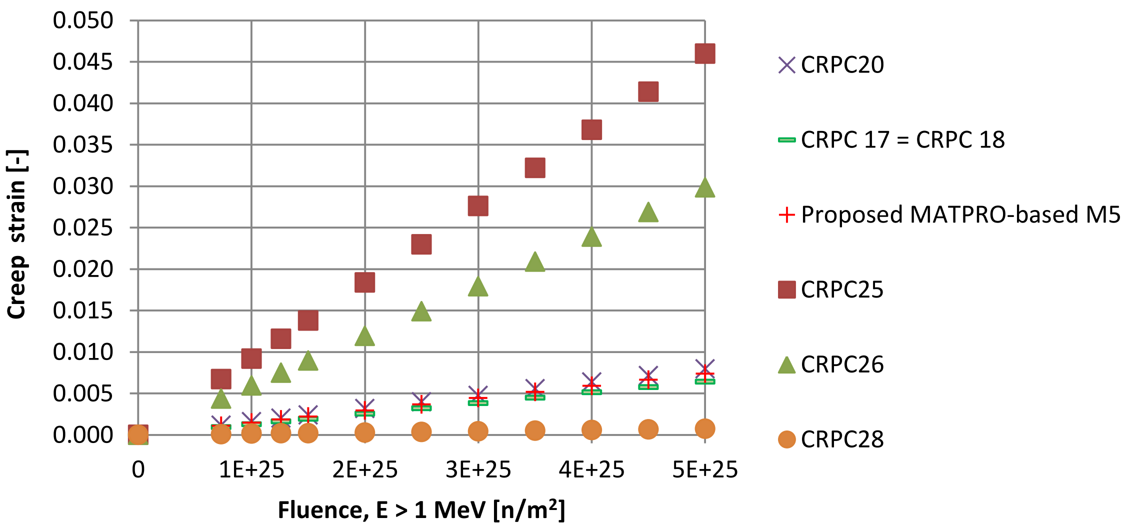

Figure 21 Comparison of creep correlations at 653.15 K and 90 MPa, (JRC-ITU 2014), (Luscher et al. 2011), (Gilbon et al. 2000)

The open literature does not contain sufficient data to create a dedicated creep rate correlation for M5 on the basis of M5 data alone. At this stage, it is therefore proposed to modify existing TRANSURANUS correlations for Zircaloy-4. Namely, as the materials are very close in their compositions, it is expected that shapes of the creep curves are close to each other, so a stress correction factor can be used to derive the creep correlation for M5 from that of Zircaloy-4 (Dunand et al. 1999).

The open literature provides experimental data on creep comparing Zircaloy-4 and M5 in different pressure and temperature conditions (Forgeron et al. 2000). Using the Larson-Miller parameter it is possible to obtain the stress correction factor, which can then be used in existing creep models for Zircaloy-4 to predict different creep behaviour of M5.

The Larson-Miller parameter (*PLM*) (Dunand et al. 1999) is calculated in Eq. 26:

$$\mathrm{PLM} = (\log t_r + c) * T \tag{26}$$

where time to rupture t_r is in hours, material constant c is dimensionless and temperature T is in Kelvin.

The material constant c is chosen in accordance with experimental data (it is typically close to 20). In our case, the best fit with the experimental data on Zircaloy-4 and M5 was obtained with a value of c equal to 11. PLM for both Zircaloy-4 and M5 as a function of stress are presented in Figure 22.

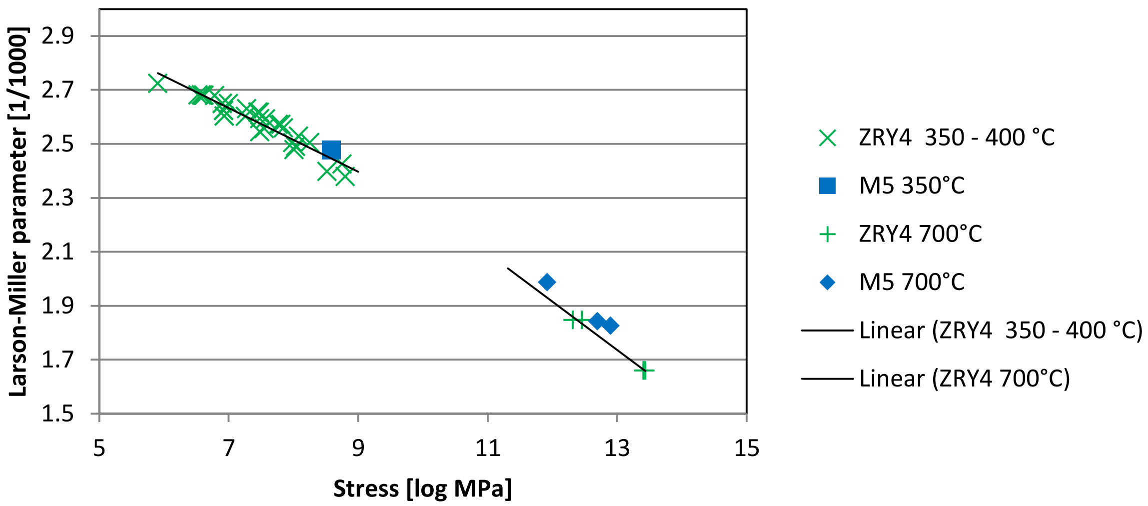

Figure 22 Larson-Miller parameter as a function of stress based on data from (Forgeron et al. 2000)

The linear fit of the Larson-Miller parameter for Zircaloy-4 allows us to predict a stress at any temperature and rupture time within the interpolated values. Material stresses for Zircaloy-4 and M5 for the same PLM can then be compared to obtain the stress correction factor, as described in Eq. 27:

$$\tau = \frac{\sigma_{ZRY4}}{\sigma_{M5}} \tag{27}$$

where σ_{ZRY4} and σ_{M5} is the stress in MPa of Zircaloy-4 and M5, respectively.

Using the above outlined approach, it was possible to obtain the stress correction factor in four experimental points out of which an average value of the stress correction factor equal to 0.879 was calculated. This was then used in creep laws for Zircaloy[14] already implemented in TRANSURANUS (No. 18 and 20) to develop M5 correlations (cf. Eqs. 28 and 29):

$$\dot{\varepsilon}_{normal} = \frac{1}{24} 2.6 * 10^6 * e^{-\frac{17000}{T}} * \sinh\left(\frac{\tau * \sigma_{eff}}{60}\right) + 2.46 * 10^{-25} * \left(\frac{145.034 * \tau * \sigma_{eff}}{1000}\right)^4 * \Phi + 2.928 * 10^{-25} * \left(145.034 * \tau * \sigma_{eff}\right) * \Phi \tag{28}$$

14 There is in general little information available about the Zircaloy cladding materials used in experiments. Therefore, TRANSURANUS sometimes does not distinguish between Zry-2 and Zry-4, even though there might be non-negligible differences.

$$\dot{\varepsilon}_{LOCA} = 3600 * a_f * \tau * \sigma_{eff}{}^{n} * e^{-\frac{q}{8.314*T}} * \frac{r_r}{r_a} \tag{29}$$

where

$\dot{\varepsilon}$	Strain rate [1/h] for nominal and LOCA conditions	n	Stress exponent
T	Temperature [K]	a_f	Structure parameter, effective
σ_{eff}	Effective stress [MPa]	r_r	Reference radius
Φ	Fast neutron flux [n/m^{2}s]	r_a	Actual radius
τ	Stress correction factor	q	Activation energy

Comparison of the proposed M5 creep correlation for operational conditions with measured data for M5 at the temperature of 653.15 K and pressure of 90 MPa (Gilbon et al. 2000) is given in Figure 23.

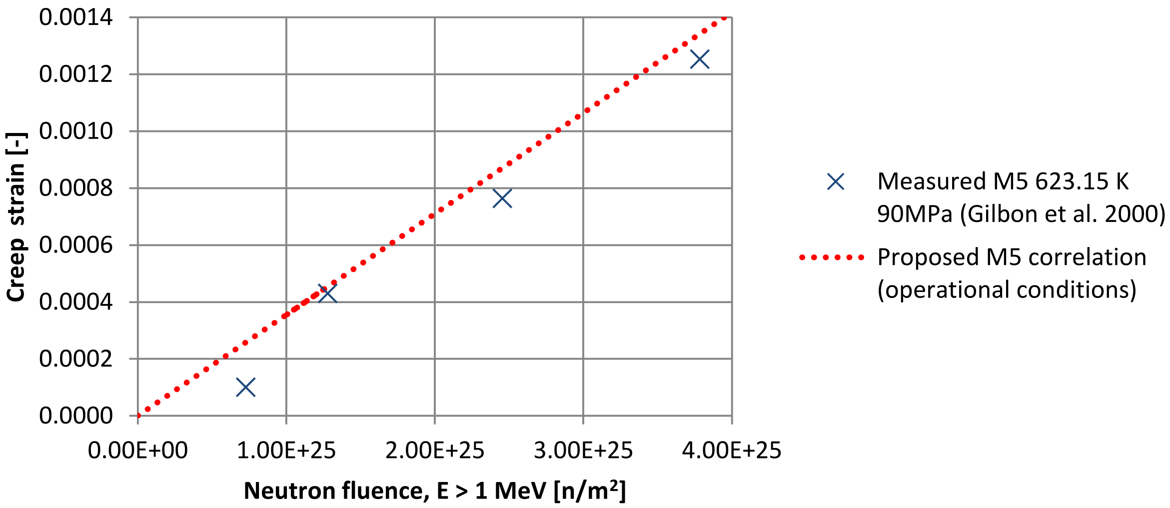

Figure 23 Comparison of the proposed M5 creep correlation with measured data for M5 at the temperature of 653.15 K and pressure of 90 MPa (Gilbon et al. 2000)

4.6.2 Conclusion

The proposed M5 correlation is deemed to be in a reasonably good agreement with the available experimental data. In most cases the proposed correlation provides slightly higher creep values. Future development should be aimed at creation of a dedicated M5 creep correlations, based on the available data (possibly also from Halden experiments) taking also into account the creep rate dependence.

In a similar way, the current creep correlation for E110, and in particular the anisotropy factors, shall be updated on the basis of more recent Russian data available in the open literature as suggested by colleagues from ÚJV in the Czech Republic.

4.6.3 Draft correlation – ETACR

The proposed M5 correlations are based on Zircaloy creep correlations already implemented in TRANSURANUS (under property numbers 18 (LOCA conditions) and 20 (normal conditions)). The modification consists of multiplication of the stress by the calculated stress factor. The changes are presented below.

```
! M5 LOCA conditions (property No. 21)
.
.      depsdt = 3600.0*af*0.879*sigv**n*EXP(-q/(8.314*tk))
.
..
```

```
. ! M5 normal conditions (property No. 22)
.
.
..     sigmap = 0.879 * sigv * 145.034

    sigman = 0.879 * sigv / 60.
.
```

4.7 Rupture Strain

Failure criteria in TRANSURANUS are specified either through the rupture strain or burst stress based on the selection of code user.

The rupture strain is considered separately in the TRANSURANUS code for the normal and loss-of-coolant (LOCA) conditions in the subroutines ETAPRR and RUPSTR, respectively (JRC-ITU 2014).

For nominal conditions two different correlations are implemented in TRANSURANUS, corresponding to LWR conditions (no. 20) and VVER conditions (no. 25). For LOCA conditions, the code contains a simple correlation applicable to Zircaloy[15] and VVER E110 cladding, no. 18 and no. 25 respectively.

4.7.1 Analysis

The correlation corresponding to nominal LWR conditions predicts the constant value of rupture strain being equal to 0.2 (cf. Figure 24). The correlation calculating rupture strain of E110 in nominal conditions is more complex as it allows the prediction of the rupture strain as a function of temperature. There is no information available about the applicability of those correlations for M5 cladding material.

For the LOCA conditions, the correlation predicts a constant engineering tangential rupture strain equal to 0.4, which is then converted to true strain as given by Eq. 30:

$$\eta = \log(1 + 0.4) \tag{30}$$

Based on the research in open literature, two sets of suitable data allowing a possible incorporation of M5 data to TRANSURANUS were found in the PROMETRA code (Cazalis et al. 2005). These two sets provide information about rupture strain of M5 as a function of temperature and burnup. Using an envelope method a new correlation for M5 corresponding to nominal conditions is proposed on the basis of these data. The proposed correlation predicts a constant value of rupture strain irrespective of temperature as described in Eq. 31. A comparison of the existing correlations in TRANSURANUS with the proposed M5 correlation is given in Figure 24.

$$\eta = 0.27 \tag{31}$$

where T is temperature in K.

[15] There is in general little information available about the Zircaloy cladding materials used in experiments. Therefore, TRANSURANUS sometimes does not distinguish between Zry-2 and Zry-4, even though there might be non-negligible differences.

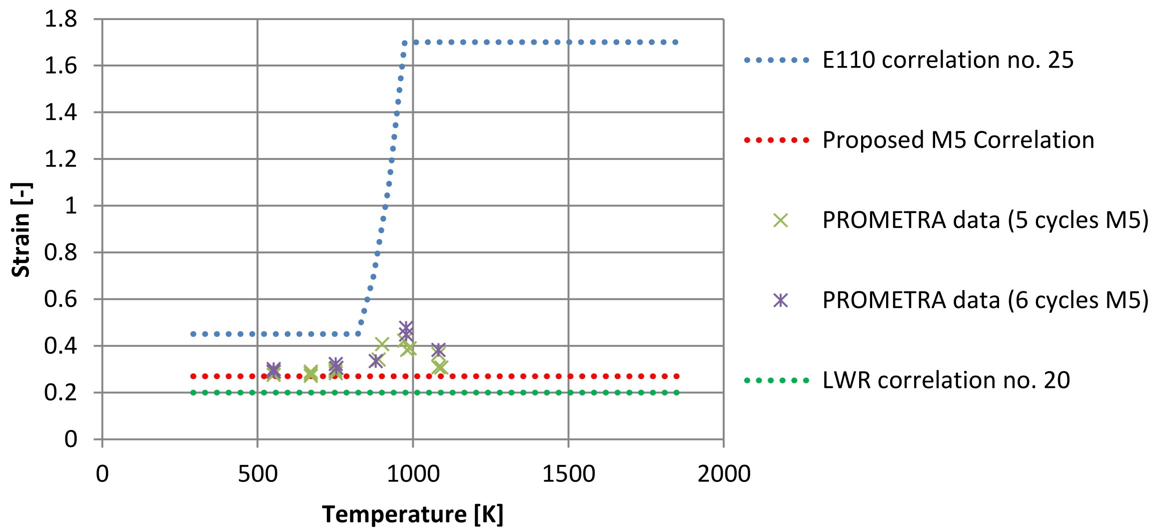

Figure 24 Rupture strain as a function of temperature in the normal conditions[16] (ETAPRR) (JRC-ITU 2014), (Cazalis et al. 2005)

There are no data available regarding the rupture strain of M5 in LOCA or other accidental situations.

4.7.2 Conclusion

The rupture strain of M5 is proposed to be adopted to TRANSURANUS on the basis of data used by the PROMETRA code. In LOCA conditions, in absence of any experimental data, the rupture strain is proposed to be calculated the same as for the other cladding materials.

The rupture strain during nominal operating conditions needs to be further investigated. The issues to clarify are: the growth of the strain in temperatures between 750.15 K to 978.15 K[17] and the decrease of the rupture strain data at ~1090 K.

Experimental data on M5 behaviour, including high temperature and irradiation effects, would be necessary to propose possibly more accurate correlation for rupture strain of M5 in LOCA and other accidental conditions.

4.7.3 Draft Correlation – ETAPRR

```
 221  continue

!    === Properties M5

      etaprr = 0.27 * Random_Var(9,4,4)

     return
!    ++++++
```

4.7.4 Draft Correlation – RUPSTR

```
 221 continue

!   M5 approximation based on Zircaloy
```

[16] The correlation no. 25 shows a decrease of E110 rupture strain in the temperature range between approx. 823 K to 973 K probably due to phase transition. However, this does not correspond to the phase transition temperatures of E110 given in TRANSURANUS (approx. 1050 K to 1173 K) (JRC-ITU 2014).

[17] This effect would rather be expected in the range of the phase transition, which occurs at higher temperatures ($t_{\alpha > \alpha+\beta}$ = 1023.15 K and $t_{\alpha+\beta > \beta}$ = 1233.15 K)

```
      rupstr0 = 0.4          ! approximation of engineering strain
!                     at rupture during LOCA in a PWR

      rupstr = rupstr0 * Random_Var (19, 4, 4)

!     Engineering to true strain conversion

      rupstr  = log(1.+ rupstr)

      return
!     ++++++
```

4.8 Burst Stress

The burst stress is considered in the subroutine SIGMAB. In the TRANSURANUS code, burst stress correlations corresponding to Zry-4 (no. 20) and E110 (no. 25) claddings are implemented (JRC-ITU 2014).

4.8.1 Analysis

Both existing correlations for Zry-4 and E110 are temperature dependent (cf. Figure 25). In addition, the oxygen embrittlement at higher temperatures and its influence on burst stress is taken into account by adoption of a reduction factor (which is calculated in the TRANSURANUS code as a function of oxygen concentration).

The proposal for the M5 correlation for burst stress has been developed on the basis of experimental data from the SKI report (Massih 2007). Burst stress values for temperatures higher than 1473.15 K, for which experimental data are not available, were extrapolated using a logarithmic fit from measured values between 1123.15 K and 1473.15 K. Logarithmic extrapolation was also used for low temperatures below 873.15 K.

The proposed M5 burst stress correlation is given in the Eqs. 32 through 35. The comparison of the existing TRANSURANUS correlations and the proposed M5 correlation for burst stress is given in Figure 25.

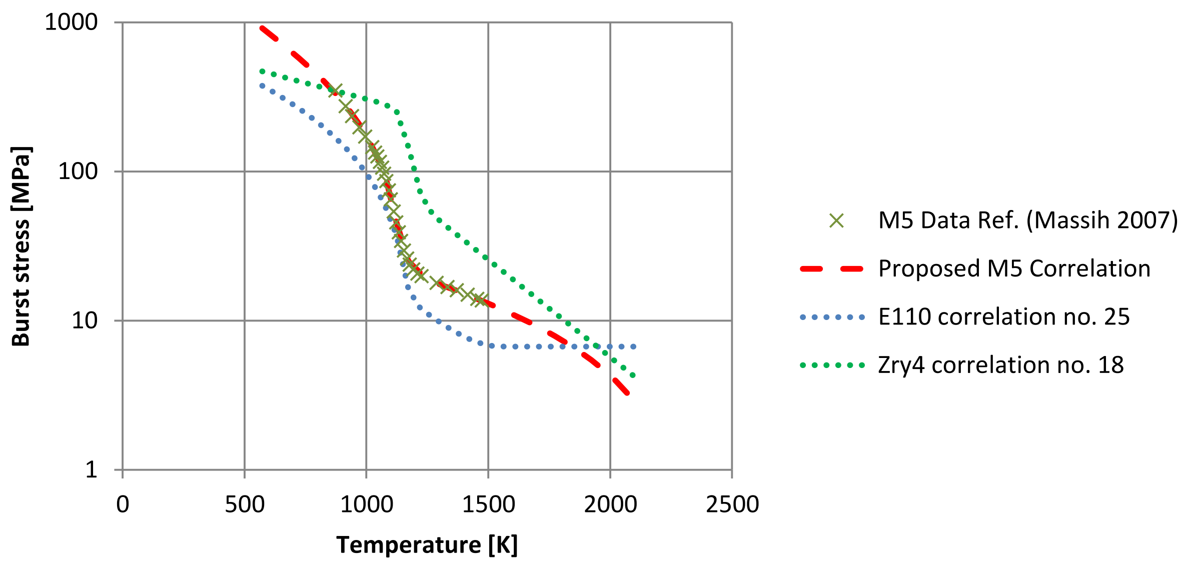

Figure 25 Burst stress as a function of temperature (JRC-ITU 2014), (Massih 2007)

$\sigma = -834.1 * \ln(T - 273.15) + 5668.3$ T ≤ 1073.15 K (32)

$= -1.0646 * (T - 273.15) + 951.86$ 1073.15 K < T ≤ 1123.15 K (33)

$= 17775.5 - 55.7852 * (T - 273.15) + 0.0584446 *$ 1123.15 K < T ≤ 1223.15 K (34)

$(T - 273.15)^2 - 0.0000204178 * (T - 273.15)^3$

$$= -25.52 * \ln(T - 273.15) + 194.51 \qquad T > 1223.15 \text{ K} \qquad (35)$$

where temperature T is in K and burst stress σ in MPa.

4.8.2 Conclusion

The developed proposal for M5 burst stress correlation is considered as a reasonable starting point for analyses and further improvements, including the possible impact of embrittlement due to irradiation, oxygen concentration and hydrogen pick up. The extrapolation to high temperature is in good agreement with the existing E110 TRANSURANUS correlation but only to approx. 1750 K. Note that at low temperatures (below 873.15 K), there is a considerable uncertainty in the modelling of the M5 burst stress, and that its value in this temperature range may possibly be overestimated. The proposed correlations thus may need to be revised, based also on the availability of additional experimental data on M5 behaviour.

4.8.3 Draft Correlation – SIGMAB

```
 221 continue

!    M5 alloy cladding
!    ===============
!....temperature tcl  is given in degree C
!    ========================
     if (tcl .LE. 800.) then
!    ========================
      Sigb0 = -834.1*log(tcl) + 5668.3
!    ==============================
     else if (tcl .LE. 850. ) then
!    ==============================
      Sigb0 = -1.0646*tcl  + 951.86
!    ==============================
     else if (tcl .LE. 950. ) then
!    ==============================
      Sigb0 = 17775.5 - 55.7852*tcl &
      + 0.0584446*tcl**2 - 0.0000204178*tcl**3
!    ==============================
     else
!    ==============================
      Sigb0 = -24.44*log(tcl) + 186.92
!    ======
     end if
!    ======
      relsigb = exp( -32.5*conox (lschni) )
      sigmab = Sigb0 * relsigb * Random_var(10,4,4)
     return
!    ++++++
```

5. Corrosion

The cladding corrosion phenomena are in the TRANSURANUS code calculated in the OUTCOR subroutine. The corrosion is separately solved for operational and high temperature states, where for high temperatures the subroutine HTCLOX is called by OUTCOR. The TRANSURANUS code presently includes several models to calculate corrosion rate for zirconium based cladding for operational conditions. All the models are listed in Table 11 (JRC-ITU 2014).

Table 11 Existing TRANSURANUS corrosion models for operational conditions (JRC-ITU 2014)

Model	Basic description
CORROS	MATPRO model for BWR and LWR conditions
OCECEK	EPRI/C-E/KWU PWR conditions
OCOCO	Corrosion according to EPRI code comparison exercise

At high temperature range, the TRANSURANUS code contains the following corrosion models, cf. Table 12.

Table 12 TRANSURANUS high temperature oxidation models (JRC-ITU 2014)

Number	Basic description
40&41	Cathcart-Pawel
42&43	Leistikow
44&45	Solyany for Zr1%Nb
46&47	AEKI BE for Zr1%Nb
48&49	Baker-Just

5.1 Analysis

Oxide layer growth depends on temperature, burnup and coolant chemistry. Data available in the open literature (Bossis et al. 2005) provide information about oxide layer growth on M5 cladding in operational/nominal conditions as a function of burnup. Based on these data a simplified burnup dependent correlation for M5 cladding corrosion behaviour is proposed using an envelope method to yield conservative estimates.

This proposal has also been developed using the operational data from American NPP's. These were chosen because of same operational conditions (temperature, chemistry, pressure). The developed correlations are given in Eqs. 36 and 37 and also displayed on Figure 26 and Figure 27.

$$\delta_{envelope} = 0.0208 * burnup^{0.6681} \qquad (36)$$

$$\delta_{average} = 0.0598 * burnup^{0.5089} \qquad (37)$$

where oxide layer thickness δ is given in μm and burnup is given in MWd/tU.

The CORROS model was chosen as a reference to compare with the M5 experimental data. The comparison given in Figure 26 shows the known characteristic of Zircaloy-4 corrosion behaviour: at high burnups (50 000 – 60 000 MWd/tU), the oxide layer thicknesses are about three to four times higher than those of M5 at the same burnup.

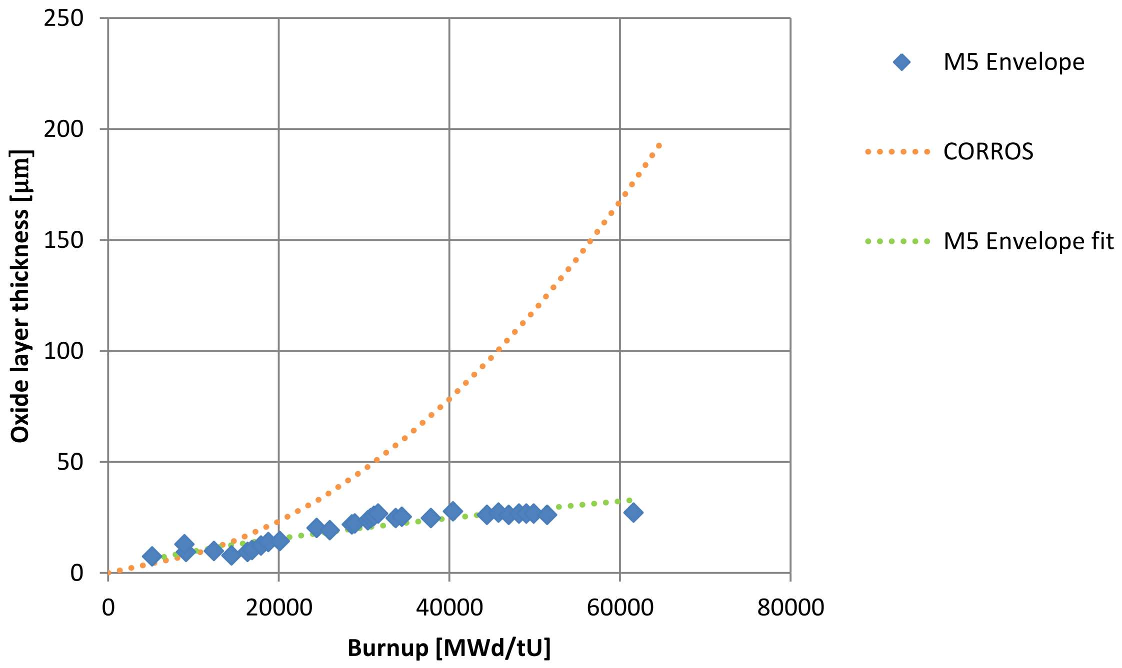

Figure 26 Comparison of the experimental M5 data and the proposed M5 correlation (envelope fit) to the existing TRANSURANUS CORROS model (JRC-ITU 2014). The comparison of M5 envelope fit (experimental data) and the predictions of the CORROS model has been made on the assumption that 1 year of operation corresponds to the burnup of 12 000 MWd/tU (Cazalis et al. 2005).

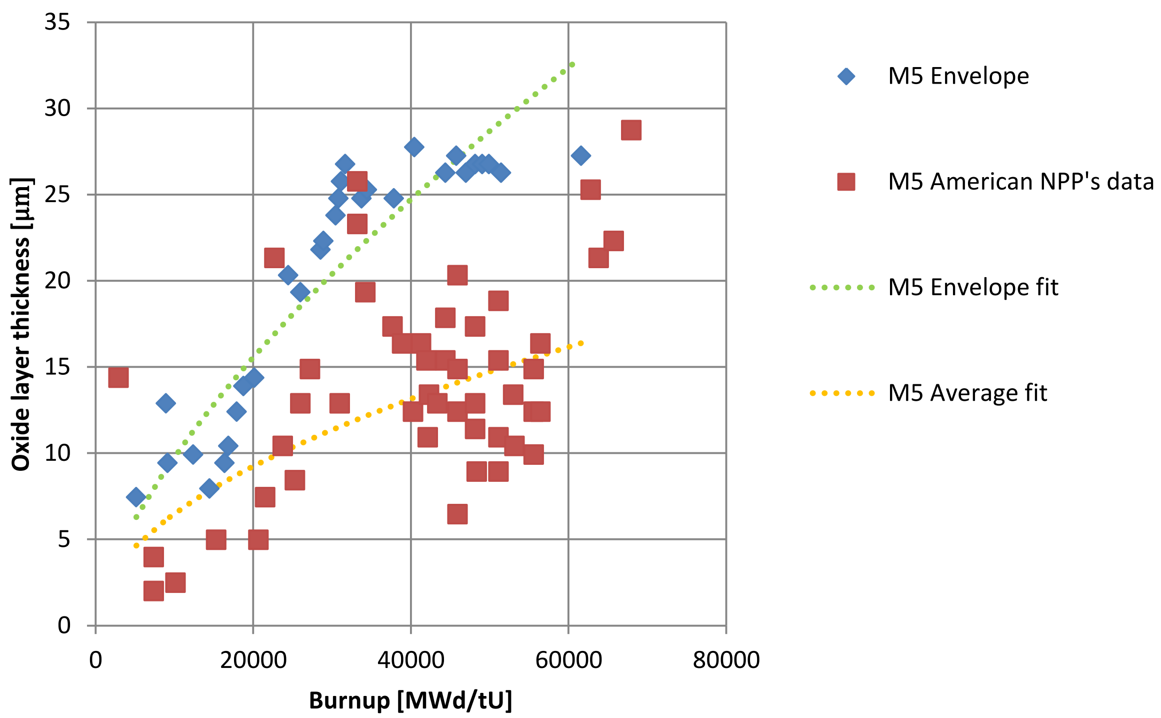

Figure 27 Comparison of the M5 experimental data and the proposed M5 correlations to predict average and envelope values of the oxide layer thicknesses.

Oxide layer thickness growth on M5 during the accidental conditions is proposed to be taken into account using a correlation based on experimental tests from (Duriez et al. 2008), cf. Eq. 38. Note, however, that the correlation is valid only for temperatures between 873 K and 1273 K.

$$K_{mass\ gain} = 1.303 * 10^{-4} * e^{-\frac{54250}{RT}} \tag{38}$$

where mass gain K is in g.mm^{-2}.s$^{-1/2}$, R is the universal gas constant, and T is temperature in K.

As TRANSURANUS needs for its calculations also the layer thickness growth rate, its correlation was obtained from the equation above, Eq. (38), using the relationship between zirconium oxide mass m_0 and oxide layer thickness δ_{ox} as given in (JRC-ITU 2014), cf. Eq. 39:

$$m_0 = \delta_{ox} * \frac{0.75}{2.85} * \rho_{Zr} \tag{39}$$

where zirconium density ρ_{Zr} is given in g/mm^3.

Using the aforesaid equations yields (in the temperature range between 873 K and 1273 K), cf. Eq. 40:

$$K_{growth\ rate} = 0.07594 * e^{-\frac{54250}{RT}} \tag{40}$$

where oxide layer thickness growth rate K is in mm.s$^{-1/2}$, R is the universal gas constant 8.3144 J/mol·K and T is temperature in K.

The comparison of the proposed M5 with the existing oxide layer thickness growth rate correlations in accidental conditions is given in Figure 28.

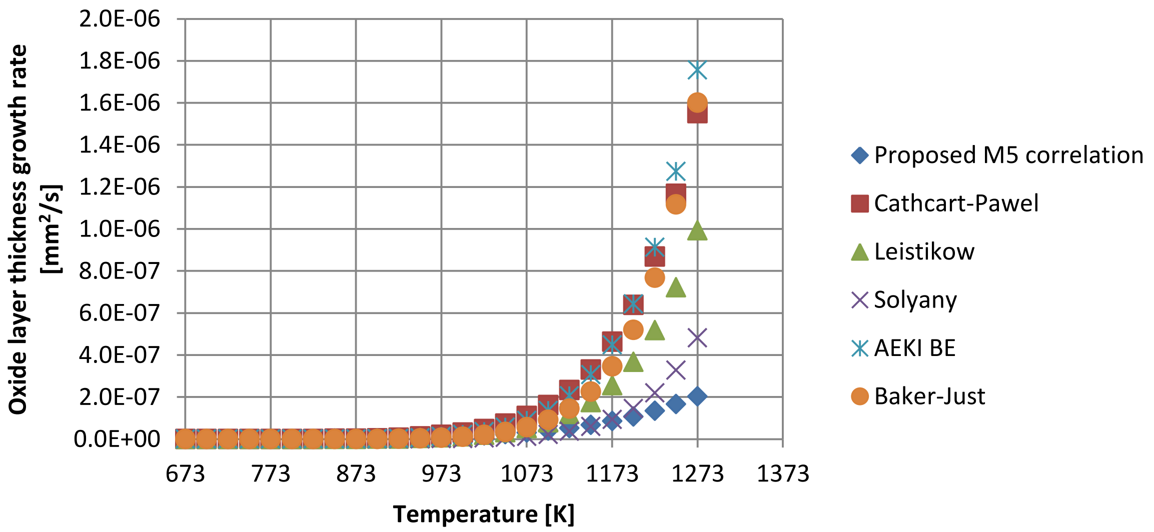

Figure 28 Comparison of the proposed M5 with the existing oxide layer thickness growth rate correlations in accidental conditions (JRC-ITU 2014).

5.2 Conclusion

The proposed M5 correlation for operational states is considered to provide conservative estimate of the oxide layer thickness of M5. It is to be noted, however, that complete information is in general not available about the exact temperature and water chemistry conditions.

Future development should therefore be aimed at gaining experimental data with more detailed operational information, cf. (Mardon et al. 2004) and (Schmidt et al. 2007). Up to now, it has not been possible to incorporate in TRANSURANUS effects of temperature, pressure or chemistry on the corrosion layer thickness. An issue of the temperature range should be further discussed to determine, which temperature should serve as an effective boundary between normal and high temperature corrosion regions. These should be aims of future development efforts.

Following the conservative approach the proposed M5 high temperature oxidation correlation is assumed to be applicable in the temperature range of 673 – 1273 K (at least), cf. Figure 28. The correlation follows the same trend as the other TRANSURANUS correlations and is also in good agreement with experimental data, as M5 has a significantly better corrosion resistance than other zirconium alloys. Future development should be aimed at the temperature range between operational states and 873 K (i.e., validity range of the high temperature corrosion correlation for M5). Nevertheless, above 1373 K (i.e., at temperatures typically calculated for LOCA), the Baker-Just correlation seems to provide conservative estimates also for M5 (Mitchel et al. 2000).

5.3 Draft Correlation – OUTCOR

```
!
!   =====================================================
    Else if ( icorro .ge. 36  .and.  icorro .le. 39 ) Then
!   =====================================================
!     M5 cladding corrosion model
!     === High temperature steam oxidation (teta >673.15 K)
!           operational data fit   (teta < 673.15 K)

!     --- Time step (s)

      dtsec = dt * 3.6d+03

!     --- Oxide-cladding interface temperature (K)

      toxcli = teta (m1, m2(m1), 1) + 273.15

!     --- Thermal conductivity of Zirconium dioxide (W/mm/K)
      loxide (lschni) = 0.002
!     loxide (lschni) = 0.835+1.8e-4*toxcli
!
!     Defining cladding weakening
!
      IF ( icorro .eq. 38 .or. icorro .eq. 36) iocmch = 0
      IF ( icorro .eq. 39 .or. icorro .eq. 37) iocmch = 1

!     *************************
      IF (toxcli .lt. 673.15) Then
!     *************************

!       --- Oxide thickness at the end of previous time step (um)

        zro2ai = soxide (lschni,2)

!       --- New oxide layer thickness (um)
        IF (icorro .eq. 38 .or. icorro .eq. 39)zro2bi = 0.0208*(burnup**0.6681)*0.001
        IF (icorro .eq. 36 .or. icorro .eq. 37)zro2bi = 0.0598*(burnup**0.5089)*0.001
        soxide (lschni,1) = zro2bi

!        --- Zirconium wall thinning (mm)
```

```
        deltcl = 2./3. * ( zro2bi - zro2ai )

!        --- Oxygen mass increment in the cladding (g/mm**2)

        delgmo = 1.125 * deltcl * 6.55e-3 / 2.85

!        --- Total Oxygen mass / cladding surface area (g/mm*2)

        gmoxi(lschni,1) = gmoxi(lschni,2) + delgmo
!      ****
      Else
!      ****
!        High temperature oxidation model
!        --------------------------------
        Call Htclox (toxcli, dtsec, deltcl)
!        +++++++++++
!      ******
      End If
!      ******

!       --- Total oxygen mass gain (g/mm)

       delgox = (gmoxi(lschni,1)-gmoxi(lschni,2))*2.*rclout*PInumb

!       --- Heat generation rate (W/mm)

       qclox(lschni) = 6.45e+3 * delgox / dtsec!--------------------------
```

5.4 Draft Correlation – HTCLOX

```
!    ============================================
    ELSE IF ( icorro .EQ. 36 .OR. icorro .EQ. 39 ) THEN
!    ============================================
!       M5 high temp correlation
!       =========================
!       OXIDE LAYER GROWTH RATE (mm**2/s)
!       ----------------------
       dlgr = 5.766884E-3 * exp(-13050./TK)
!       OXYGEN MASS GAIN RATE (g**2/mm**4/s)
!       ---------------------
       dmgr = 1.697809E-8 * exp(-13050./TK)
```

6. Additional modifications

The information about the cladding material is also included in several other subroutines, which are listed in Table 13 below. Upgraded source code taking into account the new M5 correlations is presented in following paragraphs.

Table 13 Modified TRANSURANUS read and write subroutines (JRC-ITU 2014)

Subroutine	Basic description
Beginn.f95	Reads input and writes it with comment into output
Inpt54.f95	Records some input variables
Inpt58.f95	Same as above
Inpt65.f95	Same as above

Modified subroutines are listed below.

- Beginn.f95
  - Line 141
    ```
    if ( pincha (4) .eq. 'm5c' )   pincha (4) = 'M5C'
    ```
  - Line 251
    ```
    if ( PinCha (4) .eq. 'M5C' )                  &
    Text_PinCha (4) = '(M5 cladding)'
    ```
- Inpt54.f95
  - Line 462
    ```
    If (icorro .eq. 38) write (nwrite,4138) icorro
    If (icorro .eq. 39) write (nwrite,4139) icorro
    ```
  - Line 493
    ```
     If (icorro .eq. 38) write (nwrite,4106)
     If (icorro .eq. 39) write (nwrite,4106)
    ```
  - Line 505
    ```
     If (icorro .eq. 38) write (nerror,4106)
     If (icorro .eq. 39) write (nerror,4106)
    ```
  - Line 590
    ```
       icorro .eq. 38 .or.                    &
       icorro .eq. 39 .or.                    &
    ```
  - Line 700
    ```
    4138 FORMAT (' ICORRO =',I5,5X,                     &
         'M5 corrosion model;',/,19x,  &
         'Thinning of the cladding wall is not considered'/)
    4139 FORMAT (' ICORRO =',I5,5X,                     &
         'M5 corrosion model;',/,19x,  &
         'Thinning of the cladding wall is considered in mechanics'/)
    ```
- Inpt58.f95
  - Line 160
    ```
         MatProp_clad (4) .eq. 22 .or.              &
    ```
- Inpt65.f95
  - Line 230
    ```
    If (icorro_loca .eq. 38) write (nwrite,3138) icorro_loca
    If (icorro_loca .eq. 39) write (nwrite,3139) icorro_loca
    ```
  - Line 658
    ```
    3138 FORMAT (' ICORRO_loca =',I5,5X,                &
         'M5 corrosion model;',/,24x,  &
         'Thinning of the cladding wall is not considered'/)
    3139 FORMAT (' ICORRO_loca =',I5,5X,                &
         'M5 corrosion model;',/,24x,  &
         'Thinning of the cladding wall is considered in mechanics'/)
    ```

Conclusions

The present report describes an upgrade of the TRANSURANUS code with a first set of M5 cladding material properties. Based on research in open literature, correlations describing material properties of M5 alloy were introduced and incorporated in the TRANSURANUS code. These comprised thermal, mechanical and corrosion behaviour of this cladding material in both operational and accidental conditions.

Further work will be aimed at benchmarking of the code, analysing a set of cases representative to both operational and accidental conditions and comparing the behaviour of M5 alloy to Zircaloy-4 and E110, which are already incorporated in the TRANSURANUS code. This might be followed by code validation on several Halden Reactor Project experiments, on the condition of a direct access to outcomes of these experiments.

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List of abbreviations and definitions

CWSR	Cold Worked Stress Relieved alloy
JRC	Joint Research Centre
LD	Longitudinal Direction
LOCA	Loss-of-Coolant Accident
LWR	Light Water Reactor
MATPRO	Material Property Correlations
NPP	Nuclear Power Plant
PWR	Pressurised Water Reactor
RXA	Fully Recrystallized Alloy
SRA	Stress Relief Annealed alloy
TD	Transversal Direction
VVER	Water-Water Energetic Reactor
Zry-2	Zircaloy 2
Zry-4	Zircaloy 4

List of figures

List of tables

LC-NA-28366-EN-N

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Publications Office

doi:10.2789/320793

ISBN 978-92-79-64655-3