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MODELING OF PWR FUEL AT EXTENDED BURNUP

Raphael M. Dias[1], Antonio Teixeira e Silva[2]

Instituto de Pesquisas Energéticas e Nucleares (IPEN / CNEN - SP)
Av. Professor Lineu Prestes 2242
05508-000 São Paulo, SP
[1]rmdias@ipen.br, [2]teixeira@ipen.br

ABSTRACT

Since FRAPCON-3 series was rolled out, many improvements have been implanted in fuel performance codes, based on most recent literature, to promote better predictions against current data. Much of this advances include: improving fuel gas release prediction, hydrogen pickup model, cladding corrosion, and many others. An example of those modifications has been new cladding materials has added into hydrogen pickup model to support M5™, ZIRLO™, and ZIRLO™ optimized family under pressurized water reactor (PWR) conditions.

Recently some research have been made over USNRC's steady-state fuel performance code, assessments against FUMEX-III's data have concluded that FRAPCON provides best-estimate calculation of fuel performance.

Face of this, a study is required to summarize all those modifications and new implementations, as well as to compare this result against FRAPCON's older version, scrutinizing FRAPCON-3 series documentation to understand the real goal and literature base of any improvements. We have concluded that FRAPCON's latest modifications are based on strong literature review. Those modifications were tested against most recent data to assure these results will be the best evaluation as possible. Many improvements have been made to allow USNRC to have an audit tool with the last improvements.

1. INTRODUCTION

FRAPCON is the steady-state fuel performance code from USNRC and is used in audit process to licensing vendor fuel performance code in the United States. Recent version of NRC's code has received improvements to calculate fuel behavior under high burnup.

Today, nuclear fuels in PWR reactors has experimented an extended burnup. It is expected in near future a target by 60 GWd/tU [1], which is a reasonable limit to achieve.

When a nuclear reactor fuel is operated for long times some phenomena starts to occur and can, potentially, limit life-time for the fuel rods. The literature today have been summarizing high burnup with following effects [2]: Behavior of UO_2 and Behavior of Cladding.

Behavior of UO_2 has the following phenomena playing back: Formation of high-burnup microstructure and thermal fission gas release.

Behavior of cladding has the following phenomena playing back: clad corrosion behavior and clad mechanical properties.

The complex nature of those phenomena and the difficulty to work with post-irradiated materials, brings to researchers a big barrier to step-forward, thus computational simulations have developed to facilitate the calculation of fuel behavior at high burnup.

2. FRAPCON MODELS AND CHANGES

The models present in the FRAPCON today have been modified along the years. In this section we will list those models that were changed.

2.1. Coolant Conditions

FRAPCON-3 series had coolant heat capacity changed after 3.3 version.

FRAPCON-3 heat capacity was calculated using the following relationships [3]:

$$C_p = 2.4x10^5 (J/Kg).K \; for \; T_b(z) < 544\,K \tag{1}$$

$$C_p = 2.4x10^5[1 + 2.9x10^{-3}(1.8\,T_b(z) - 1031)] \; for \; 544\,K \le T_b(z) < 588\,K \tag{2}$$

$$C_p = 2.4x10^5[1 + 2.9x10^{-3}(1.8\,T_b(z) - 979.4)] \; for \; T_b(z) \ge 588\,K. \tag{3}$$

FRAPCON 3.3 until the latest version 3.5 calculates heat capacity using the following relationships [4], [5]:

$$C_p = 2.39x10^5 (J/Kg).K \; for \; T_b(z) < 544\,K \tag{4}$$

$$C_p = 2.39x10^5[1 + 7.73x10^{-4}(1.8\,T_b(z) - 979.4)] \; for \; 544\,K \le T_b(z) < 583\,K \tag{5}$$

$$C_p = 2.39x10^5[1 + 2.95x10^{-3}(1.8\,T_b(z) - 1031)] \; for \; T_b(z) \ge 583\,K. \tag{6}$$

2.2. Conduction through the Interfacial Gas

The FRAPCON's expression to calculate the conductance due to conductive heat transfer through the gas in the fuel-cladding is the same since version 3.0, but recently in version 3.5 the internal constant A has changed from A=0.7816 [3], [4] to A=0.0137 [5].

2.3. Conduction through Points of Contact

The model of contact conductance in the FRAPCON series is a modification [3], [4], and [5], of the Mikic-Todreas [6], model.

Into the FRAPCON 3.3 the model used was:

$$h_{solid} = \frac{5.0K_m P_{rel} R_{mult}}{RE}, if\ P_{rle} > 0.003 \tag{7}$$

$$h_{solid} = \frac{0.015K_m}{RE}, if\ 0.003 > P_{rel} > 9x10^{-6} \tag{8}$$

$$h_{solid} = \frac{5.0K_m P_{rel}^{0.5}}{RE}, if\ Prel < 9x10^{-6} \tag{9}$$

$$E = exp[5.738 - 0.528\ ln(R_2)]. \tag{10}$$

Those relationships into both the FRAPCON-3.4 and 3.5 have changed to:

$$h_{solid} = \frac{0.4166K_m P_{rel} R_{mult}}{RE}, if\ P_{rle} > 0.003 \tag{11}$$

$$h_{solid} = \frac{0.00125K_m}{RE}, if\ 0.003 > P_{rel} > 9x10^{-6} \tag{12}$$

$$h_{solid} = \frac{0.4166K_m P_{rel}^{0.5}}{RE}, if\ Prel < 9x10^{-6} \tag{13}$$

$$E = exp[5.738 - 0.528\ ln(3.937x10^{7} R_f)]. \tag{14}$$

2.4 Radial Power Profile

The radial power profile model was added on the FRAPCON-3.3 [12] and uses this model to calculate radial power profile in UO_2 and MOX under LWR and HWR [4], [5]. The internal code function TUBRNP is based on Lassman model [4] , [5].

Lassman investigated the dependence of the radial power density q''' on the burnup which is basically determined by the fuel rod geometry, the initial concentration of fissile material and the Pu buildup [7].

The Lassman model predicts the radial power density distribution of fuel pellet as a function of burnup and radial burnup profile as a function of time, the model was considered as an evolution of the Palmer's RADAR model and was used in TRANSURANUS code [7].

USNRC's code is not able to calculate radial power profile under urania-gadolinea fuel, to calculate power profiles for this type of fuel FRAPCON uses interpolated values from a table [4], [5].

2.5 Thermal Conductivity and Iteration Procedures

The fuel thermal conductivity has been investigated for long time and it is an important property of high burnup fuel behavior. It has been influencing the uranium dioxide pellet operating temperature and many studies [9, 10], have point out that thermal conductivity degradation is affected by burnup process due to radiation damage, solid fission product and fuel gas bubble formation.

The USNRC's thermal analysis code model presented in the FRAPCON-3.0 was based on model developed by Lucuta and the expression included the Harding and Martin term [3].

In the FRAPCON-3.3 model used in 3.0 version was abandoned and replaced by another expression developed by Nuclear Fuel Industries (NFI) the [Ohira and Itagaki, 1997] model, with modifications made by PNNL (Pacific Northwest National Laboratory), NFI model is de facto standard in FRAPCON series and its use is recommended [12].

The FRAPCON documentation do not provide good physics arguments about the modification term which PNNL introduced into [Ohira and Itagaki, 1997] model: $(1 - 0.9\exp(-0.04\mathrm{Bu}))$. The paper [Unal, Stull, Willians, 2013] have discussed the PNNL modification and the modification's genealogy which resulted in recently thermal conductivity model.

The code has another thermal conductivity model, in respect at the request of the NRC, the second expression is the Halden MOX fuel model developed by the Halden Reactor Project and was first introduced in the FRAPCON-3.2, PNNL has not verified this model, but despite of this, Halden Reactor Project staff has verified the model against your set of in-reactor MOX fuel data [12].

2.6 Extension to Creep

The method of solution used in FRAPCON-3 series is the model described by Limbäck and Anderson [4], use the thermal creep model described by Matsuo [4], tuned model parameters given by Franklin [4] and modifications made by PNNL staff. Due to complex explanation which goes beyond the scope of this paper and can be found on the US-NRC docs [3], [4], [5], [12], we will only make some points out of the modification's base.

The documentation of extension to creep model which was presented in the FRAPCON-3 series did not mention exactly whether other Zircaloy alloys were supported [3].

In the FRAPCON-3.3 the model was changed with the introduction of Zirlo™ and M5™ support[12] in code's version 3.4 and 3.5, the extension creep model has the most complex expression which has different parameters for Zircaloy-4 and Zircaloy-2, the cladding the stress relief annealed (SRA) and re-crystallized annealed (RXA) equations[4], [5]. Both FRAPCON-3.4 and 3.5 version, internally select RXA's correlation for M5™ and SRA's correlation for ZIRLO™ and ZIRLO™ Optimized which is reduced by a factor of 0.8 for SRA [4], [5].

The FRAPCON-3.5 model for extension creep has one modification against 3.4 version, in the strain rate expression, which is calculated based on the time since the last stress has changed more than 5MPa [5].

2.7 Radial Deformation

In the FRAPCON-3.5 the radial deformation has received a gaseous swelling model based on data from Mogensen [13], who performed a irradiation test in the OECD Halden reactor using a Danish fuel assembly IFA 148 and concluded that the gas released during a power transient is followed by restructuring of the fuel [13]. FRAPCON developer team, in accordance with other authors [8], [9], [13], have believed that those test suggested gaseous swelling affect UO_2 pellets and may influence permanent cladding hoop strain in extended burnup fuel rods [5]. The following expressions govern the model which are phased in between 40 and 50 GWd/MTU by applying a factor that varies linearly between 0 and 1 [5].

$$\frac{\Delta l}{l} = 4.55x10^{-5}T - 4.37x10^{-2} \ \ (960°\mathrm{C} < T < 1370°\mathrm{C}) \tag{15}$$

$$\frac{\Delta l}{l} = 4.05x10^{-5}T - 7.40x10^{-2} \ \ (1370°\mathrm{C} < T < 1832°\mathrm{C}). \tag{16}$$

2.8 Fuel Relocation

FRAPCON uses, since 3's version, GT2R2 model was developed by Cunningham and Beyer. This model is almost the same as the Oguma's model [16] but less complex [5].

The model used FRAPCON (Berna et al. 1997) is in fact almost the same model than was used in 3's version, FRAPCON [15] received some simple modifications in equations constants, but the operation's interval of each equation was retained and this model was used up to FRAPCON-3.4 [4].

In the FRAPCON-3.5 the fuel relocation model was more deeply updated, due to an assessment ran against 3.4's version, which have noted an under-prediction of the centerline temperatures during the first ramp to power [5]. As previous model have an excellent centerline temperature predictions throughout life this 3.4's model was retained beyond 5 GWd/MTU [5].

So, in FRAPCON-3.0 we had [15]:

$$\frac{\Delta G}{G} = 30 + 5\,FBU\;for\;LHGR < 20\frac{kW}{m} \tag{17}$$

$$\frac{\Delta G}{G} = 30 + PFACTOR + (5 + PFACTOR)FBU\;for\;LHGR < \frac{40kM}{m} \tag{18}$$

$$\frac{\Delta G}{G} = 35 + 10\,FBU\;for\;LHGR < 40\frac{kW}{m}. \tag{19}$$

In FRAPCON (Berna et al. 1997) we had some constant's modifications [3]:

$$\frac{\Delta G}{G} = 30 + 10\,FBU\;for\;LHGR < 20\frac{kW}{m} \tag{20}$$

$$\frac{\Delta G}{G} = 28 + PFACTOR + (12 + PFACTOR)FBU\;for\;LHGR < \frac{40kM}{m} \tag{21}$$

$$\frac{\Delta G}{G} = 32 + 18\,FBU\;for\;LHGR < 40\frac{kW}{m}. \tag{22}$$

Where for both models above:

$$FBU = \frac{BURNUP}{5}\;for\;BURNUP < \frac{5GWd}{MTU} \tag{23}$$

$$FBU = 1.0\;for\;BURNUP > 5\frac{GWd}{MTU}. \tag{24}$$

In the FRAPCON-3.5 we had [5]:

$$\frac{\Delta G}{G} = 0.055 \; for \; burnup < \; 0.0937 \frac{GWd}{MTU} \tag{25}$$

$$\frac{\Delta G}{G} = 0.055 + mim(reloc, reloc.(0.5795 + 0.2447 \ln(burnup)) \; for \; burnup > \frac{0.0937GWd}{MTU}. \tag{26}$$

Where:

$$reloc = \begin{cases} 0.345 \; P < 20 \\ 0.345 + \frac{P-20}{200} \; 20 \; \leq P \; \leq 40 \\ 0.445 \; P > 40 \end{cases} \tag{27}$$

2.9 Modifief Forsberg-Massih Model

The Forsberg-Massih model remains unchanged except for a small change to the diffusion constant and FITMULT into grain boundary accumulation and re-solution [5].

Into grain boundary accumulation and re-solution the FITMULT, an empirical multiplier, was changed from 250 since FRAPCON-3 to 300 in FRAPCON-3.3 [12].

In the FRAPCON-3.3 into the diffusion constant, the burnup enhancement factor was changed in opposition to 3.0 version [12]. Where in FRAPCON-3 we had an applied multiplication factor of 14 in the burnup-enhanced diffusion constant as a final step and the burnup enhancement factor had the form [3]:

$$100^{\frac{BURNUP-21}{35}} \tag{28}$$

Since FRAPCON-3.3 we have the factor multiplier changed to 12 and the burnup enhancement factor has the form [12]:

$$100^{\frac{BURNUP-21}{40}} \tag{29}$$

In the FRAPCON-3.4 the resolution parameter was changed to [4]:

$$300x1.84x10^{-14} = 1.47x10^{-12} \tag{30}$$

Against the form bellow found in FRAPCON-3.0 [3]:

$$250x1.84x10^{-14} = 1.47x10^{-12} \tag{31}$$

In the FRAPCON-3.5 in diffusion constant of Massih model above 1850K, the diffusion constant calculated at 1850K is used [5].

2.10 FRAPFGR Model

This model was added to FRAPCON-3.4 to initialize the transient release model in the FRAPTRAN and has recently been developed by PNNL staff [4].

2.11 Fuel Rod Void Volume

The fuel rod void volume is the same as the FRAPCON-3, the only little modification which include the chamfer volume in the pellet dish volume in the portion of the hot interpellet volume [5].

2.12 Waterside Corrosion and Hydrogen Pickup

The FRAPCON-3's model for waterside corrosion and hydrogen pickup both have been modified along with the USNRC's code updates. Those changes have added support for new cladding materials and improving result predicted.

Despite the fact of those modifications, the model remains the same and the FRAPCON-3.3 has only received empirical corrections in its Zircaloy-4's corrosion and hydrogen pickup model, as

PNNL staff has explained in its documents [12]. The support for ZIRLO™ and M5™ which was added to 3.3 version was only a correction value which reduces the final results of corrosion and hydrogen pickup by a factor.

In the FRAPCON-3.3 for ZIRLO™ the results calculated by the FRAPCON-3's Zircaloy-4 corrosion model was reduced by a factor of 2.0 and those predictions were closely to the ZIRLO corrosion data presented by Knott [12].

For the M5™ in the 3.3 version the FRAPCON-3's Zircaloy-4 results were reduced by a factor of 2.3 and this change made the results closely to the M5™ corrosion data presented by Mardon and Waeckel and on FRAMATOME website [12].

In the FRAPCON-3.3 the Zircaloy-4, under PWR, equation was obtained integrating, without regard to the feedback between oxide layer thickness and oxide metal interface temperature, the Garzarolli equation [4].

Into FRAPCON-3.4 the transition to thickness was attainted and a flux-dependent linear rate law was applied, because there is significant feedback between oxide-layer thickness and oxide-metal interface temperature and the oxide thickness is converted to weight gain; the approximate integral solution from Garzarolli is used [4].

Because of those modifications, after FRAPCON-3.4 the waterside corrosion model was very improved against 3.3 version as a result we had a new calculation way and not only results reduced by a factor.

In the FRAPCON-3.4 for M5 under PWR conditions we have:

$$\begin{cases} Q1 = 27446\ \left(\frac{cal}{mol}\right) \\ Q2 = 29816\ \left(\frac{cal}{mol}\right) \end{cases} \tag{32}$$

For ZIRLO we have:

$$\begin{cases} Q1 = 27446\ \left(\frac{cal}{mol}\right) \\ Q2 = 27080\ \left(\frac{cal}{mol}\right) \end{cases} \tag{33}$$

In the FRAPCON-3.5 for ZIRLO™ and ZIRLO™ optimized, under PWR conditions, the Q1 and Q2 values have changed:

$$\begin{cases} Q1 = 27080 \left(\frac{cal}{mol}\right) \\ Q2 = 27354 \left(\frac{cal}{mol}\right) \end{cases} \tag{34}$$

Into FRAPCON-3 and 3.3 the hydrogen pickup fraction was a factor set at 15%, based on data from burnup PWR rods [3] [12].

In the FRAPCON-3.4 the hydrogen pickup fraction for M5™ and ZIRLO™ was added and the fractions is respectively 0.10 and 0.125 [4].

For BWR conditions into FRAPCON-3.4 the burnup-dependent hydrogen concentration model for Zircaloy-2 was changed. For Zircaloy-2, prior to 1998, when the vendors did not have tight control over concentration and second-phase precipitate particle size the following relations are used [4]:

$$\begin{cases} H_{conc} = 47.8\, exp\left(\frac{-1.3}{1+BU}\right) + 0.316BU\ if\ BU < 50\frac{GWd}{MTU} \\ H_{conc} = 28.9 + \exp^{\left(0.177(BU-20)\right)}\ if\ BU > 50\frac{GWd}{MTU} \end{cases} \tag{35}$$

For modern Zircaloy-2, since 1998, when the vendors have had tight control over concentration and second-phase precipitate particle size the following equation used is:

$$H_{conc} = 22.8 + \exp(0.177(BU-20)) \tag{36}$$

Into FRAPCON-3.5 the hydrogen pickup fraction for M5™, ZIRLO™ and Optimized ZIRLO™ have changed to new factors and they are: for M5™ 0.10 and both ZIRLO™ and Optimized ZIRLO™ 0.175 [4].

3. CONCLUSIONS

We have concluded FRAPCON series' changes have been made based strongly on literature and PNNL staff have conducted the proper assessments to provide comparisons against the available data. The models added to support high burnup have been changed during those updates to improve the results against the most recent data.

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