RESEARCH REPORT

VTT-R-08464-11

Characterization of a representative VVER-440 fuel rod with the statistical ENIGMA

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Confidentiality: Public

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Summary

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Aim of this work was to determine the properties of a "representative rod" at various points of its reactor life. Another aim was training of fuel performance analysis. Plan was to perform several calculations with the statistical Enigma and characterize representative fuel rod in such a way, that data can be utilized e.g. in reactor dynamic codes.

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Contents

1 Introduction

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Aim of this work was to determine the properties of a "representative rod" at various points of its reactor life. Another aim was training of fuel performance analysis.

Plan was to perform several calculations with the statistical ENIGMA, and characterize representative fuel rod in such a way, that data can be utilized e.g. in reactor dynamic codes. At the moment heat transfer in gas gap is modelled in the TRAB-3D and HEXTRAN with given gas gap conductance and constant gap width. It should be considered, that the reactor dynamic codes are used in modelling of transients with period from seconds to some hours maximum. Accidents and e.g. number of damaged fuel rods are outside the scope of the dynamic codes.

2 Statistical version of the ENIGMA code

2.1 Renewal of the statistical ENIGMA

VTT has a statistical version of the ENIGMA code [1],[2], that has been used for the fuel performance analysis of different type of fuel assemblies. Development and maintenance of the ENIGMA code has branched thus that all updates of the standard ENIGMA have not been implemented to the statistical version.

In this work statistical calculations have been made in different way than previously in statistical fuel performance analysis. In normal statistical calculation certain amount of fuel rods are randomly selected from each assembly of the core, and power history of those selected rods has been used in ENIGMA calculations. In this work one common "typical" power history with variations has been used in all calculated cases. Other input parameters as design and modelling parameters can be varied in the both cases.

The existing statistical ENIGMA did not work as such at VTT's linux cluster due to the different operating system, and some work was needed in any way. At the same time of this work, VTT's standard ENIGMA was transferred to the linux cluster. To facilitate further maintenance of the statistical ENIGMA, a new

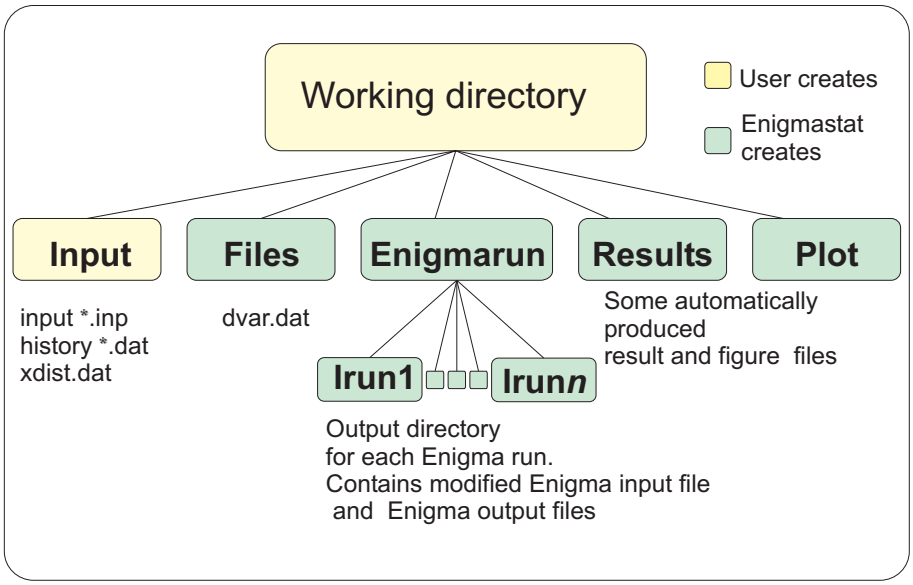


Figure 1: **The directory tree for the using of the statistical ENIGMA.**

program for statistical calculations was written with perl language. This program takes care of the input variations, performs ENIGMA calculations and also does some post-processing of results. The *Enigmastat* program performs calculations with the VTT's standard ENIGMA version. Also other corresponding fuel performance codes could be used instead of ENIGMA with minor modifications in the perl program. Enigmastat program is based on the corresponding script made for the reactor dynamic codes TRAB-3D and HEXTRAN [3].

In this work *Enigmastat* script has been used with one power history. Possibility to use several power histories from different fuel rods of core has been implemented, but not properly tested. Probably some changes in coding are still needed before *Enigmastat* works similarly to the old statistical ENIGMA code. Also statistically correct way to select fuel rods should be revised in cases, where fuel assembly includes different type of fuel rods.

2.2 Instructions for the *Enigmastat*

Structure of directory tree is shown in Figure 1. User creates directory *Input* and three input files: ENIGMA input file, file including power history and file for parameter variations. All other directories and necessary files are created by program *Enigmastat*.

ENIGMA input file **.inp* is otherwise normal input file without history input part, but varied parameters are replaced in the input by string XXXDVARiX where i is number. Power history is given in separate file **.dat* in format where three

Table 1: **Type numbers for varied parameters in file xdist.dat**

Number	type	Description
1	value	in input file string $XXXDVARiX$ is replaced by generated value
2	coefficient	in input file string $XXXDVARiXy$ is replaced by value y*generated coefficient
3	coefficient for the whole line	in input file all items of the line beginning with string XXXDVARiX are multiplied by generated value.

lines corresponds for each time step: one line for time value, one for temperatures and one for linear powers as shown below. ENIGMA calculation is made for each given time step.

Example of the format of power history file:
$time_1$
$T_1\ T_2\ T_3\ \ldots T_n$
$P_1\ P_2\ P_3\ \ldots P_n$
$time_2$
$T_1\ T_2\ T_3\ \ldots T_n$
$P_1\ P_2\ P_3\ \ldots P_n$
...

For the parameter variations file *xdist.dat* is needed. *Enigmastat* program generates parameter values for each ENIGMA run according to the data given in this file, and writes them to the file *dvar.dat*. Format of the file *xdist.dat* is following:

Name1 *Type* *Distribution* *Distribution_parameters(2-n)*
Name2 *Type* *Distribution* *Distribution_parameters(2-n)*
...

Name of the parameter is one string, no whitespaces. Alternatives for the parameter type are shown in table 1. Available distributions are shown in table 2. Number of distribution parameters and their meaning depend on the selected distribution.

The program *Enigmastat.pl* is started by giving the name and path of the script. The program asks the names of the input files, the number of calculations, and which parts of the analysis will be made. With the *Enigmastat* it is possible e.g. only generate input parameters, plot results for existing results or recalculate with earlier generated input parameters.

For the post-processing of results the script *poimi_pisteet.pl* was written. With that script it is possible to gather selected results from the ENIGMA output files

Table 2: **Distribution types and parameters given in the file xdist.dat. Types of the distributions are selected by using abbreviations of the first column in the file xdist.dat.**

Abbr.,	Distribution	Number of parameters	definition of parameters
UNI	uniform	2	minimum and maximum
DISCR	discrete	n	possible values, each of them have same probability $\frac{1}{n}$
NORM1	normal	2	limits of 95 % confidence interval
NORM2	normal	2	mean and standard deviation
STEP		1+2*number of intervals	lower limit, proportion in this interval, upper limit, proportion and upper limit are repeated for each interval
TRI	triangle	3	minimum, top and maximum

of all ENIGMA runs, e.g. value of some output parameter in each axial level and each time step, value only at single axial level at each time step, value only at selected time steps etc. The script shows instructions, if it is run without any arguments.

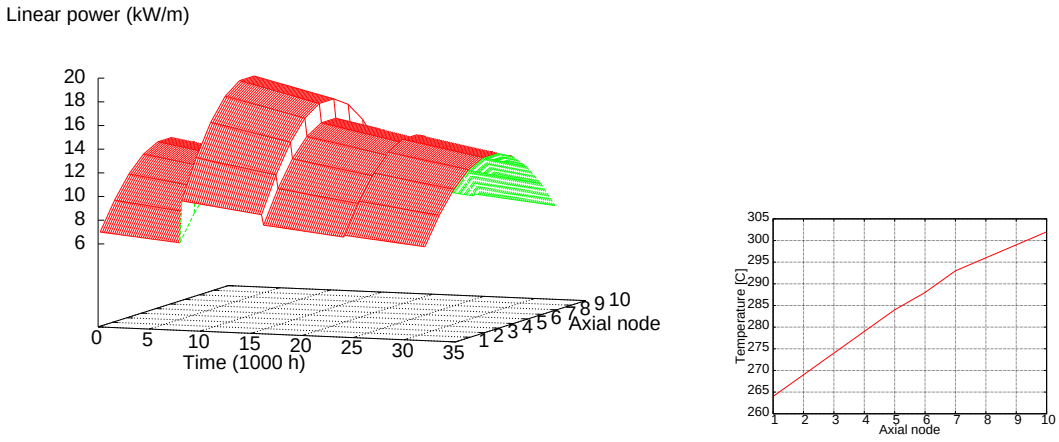
3 Analysis for the VVER fuel rod

VVER440 fuel rod was selected as a test case. Instead of real power history, artificial history was created. In the axial direction, symmetric power profile with cosine form was used. Linear power rate was highest in the second cycle and decreased linearly with time, Figure 2a. Temperature distribution was constant at each time step, Figure 2b.

Power history values were multiplied by random value between 0.8 and 1.2. Multiplier was same for each node and each time step in one ENIGMA run, but different value was used for each ENIGMA run. This multiplier describes different rods. In addition to that multiplier, each value was multiplier by value between 0.95 and 1.05. This multiplier was generated separately for each time step and it describes the uncertainty of power history data.

Input parameters were based on the values given in IAEA report [4]. Part of the input values are shown in the table 3. Set of 100 ENIGMA runs was calculated several times, e.g. with different range of varied parameters.

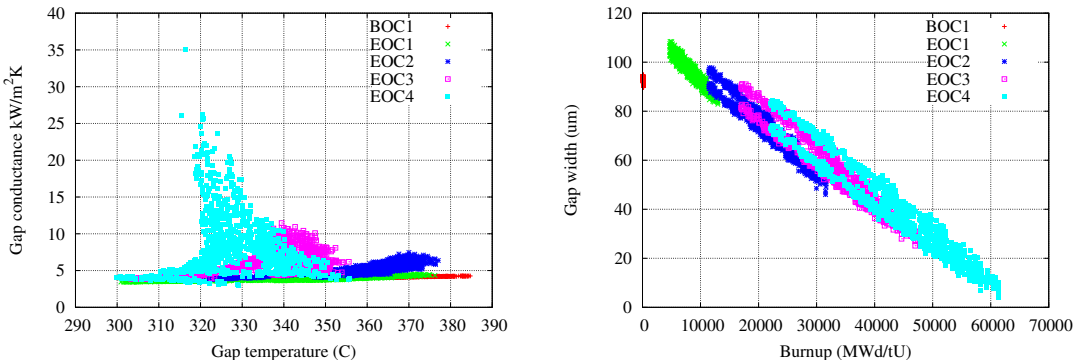
On the basis of figure 3 and other alike figures, width of the gas gap was selected as a primary output parameter. Thus aim was to represent gap width as a



(a) Power history

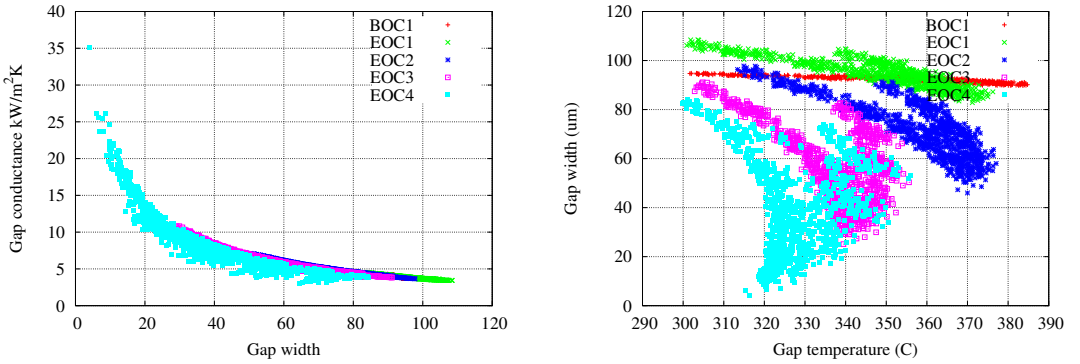
(b) Coolant temperature

Figure 2: **Rod history given as an input**



(a) Gas gap conductance as a function of gap temperature

(b) Width of gas gap as a function of burnup



(c) Gas gap conductance as a function of width of the gas gap

(d) Width of the gas gap as a function of gas gap temperature

Figure 3: **Gas gap properties of fresh, 1-year, 2-year and 3-year old fuel, calculated by ENIGMA.**

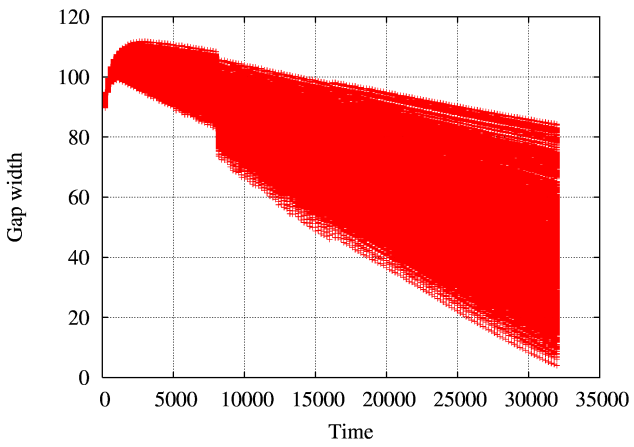


Figure 4: **Gap width as a function of time in all ENIGMA calculations.**

Table 3: **Varied input parameters and their distributions. Parameters marked with * have a constant value in figures of this report.**

Description	ENIGMA parameter	Value
1 Pellet inside radius	RIP0	$\mathcal{N}$, 95 % $\in$[0.7 mm, 0.8mm]
2* Pellet outside radius	RSP0	$\mathcal{N}$, 95 % $\in$[3.765mm, 3.785mm]
3* Cladding inside radius	RIC0	$\mathcal{N}$, 95%$\in$[3.86mm, 3.895mm]
4 Cladding outer radius	RSC0	$\mathcal{N}$, 95%$\in$ [4.525mm 4.575mm]
5 Fuel grain size		$\mathcal{N}$,95 %$\in$[10.0μm 15.0μm]
6 Helium filling pressure	PFILL	$\mathcal{N}$, 95 %$\in$[0.5, 0.6]
7 Fuel porosity	SINTPO	$\mathcal{N}$, 95%$\in$[0.016, 0.02]
8 Fission gas release	DFACT1	$\mathcal{N}$ (1.0, 0.3^2)
9 Fuel conductivity	KF(8)	$\mathcal{N}$,95%$\in$[0.04, 0.12]
10* Multiplier for cladding creep parameter	x*CRPC(5)	Unif (0.5, 1.5)

function of the burnup. Outer radius of fuel pellet and inner radius of cladding are modelled separately.

3.1 Fuel pellet radius

ENIGMA calculations were repeated so that between cycles there where cold time steps with constant 20 ^{o}C coolant temperature and with zero linear heat rate. Some cold time steps were added also during the first cycle to get more data about behaviour of fuel rod during first cycle. Test calculations show that difference in the manufactured value of pellet radius remains during the whole calculated period. Thus initial radius of fuel pellet was kept constant when ENIGMA calcu-

lations for the fitting of curve were made, and value was included as a multiplier to the equation.

The equation 1 was fitted to the calculated fuel pellet outer radius values at the cold state. In this report thermal expansion was modelled with the equation 2, but it could be taken into account only in the reactor dynamic codes. If thermal expansion is modelled in the reactor dynamic codes, also behaviour during a transient can be considered.

$$R(Bu) = R_0(a_1 e^{\frac{Bu}{a_2}} + a_3 + a_4 Bu) \tag{1}$$

R_0 in equation 1 is manufactured fuel pellet radius, Bu burnup [MWd/tU] and a_i parameters. When equation 1 was fitted to the results of the ENIGMA, following values were found for the parameters a_i:

$$\begin{aligned} a_1 &= 0.00630 \\ a_2 &= 600.0 \\ a_3 &= 0.99371 \\ a_4 &= 2.45878 \cdot 10^{-7} \end{aligned}$$

MATPRO [5] has the following representation for the thermal expansion of the fuel pellet:

$$\frac{\Delta L}{L} = k_1 T_K - k_2 + k_3 e^{-\frac{E_D}{k_b T_K}} \tag{2}$$

where K_i and E_D are parameters, k_B Boltzmann's constant and T_K temperature in Kelvins. For the UO_2 following parameter values were given:

$$\begin{aligned} k_1 &= 1.0 \cdot 10^{-5} \\ k_2 &= 3.0 \cdot 10^{-3} \\ k_3 &= 4.0 \cdot 10^{-2} \\ E_D &= 6.9 \cdot 10^{-20} \end{aligned}$$

Third term of the equation 2 is negligible at temperatures $T_K < 1000K$. Because temperature range in these calculations is below that limit, it was set $k_3 = 0$.

In the Figure 5 is shown the outer radius of fuel pellet calculated with the ENIGMA code and with equations 1 and 2 in corresponding points. Thermal expansion was calculated with average temperature of fuel pellet at particular axial level. It can be seen that equations 1 and 2 slightly overestimate the fuel radius at higher burnup points. In the ENIGMA instantaneous linear expansion coefficient according to the equation 3 is used.

$$\alpha = \alpha_1 + \alpha_2 T_K + \alpha_3 T_K^2 \frac{1}{K} \tag{3}$$

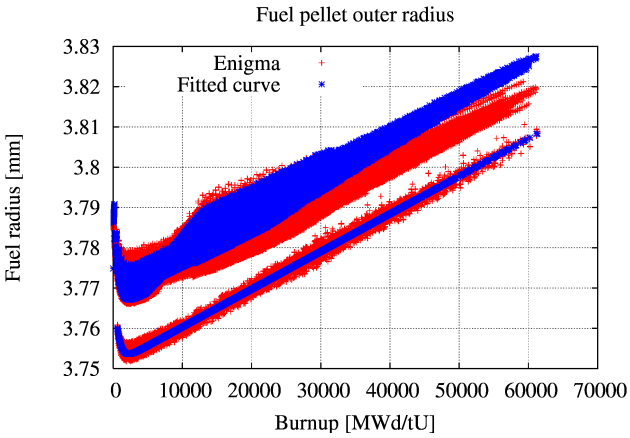


Figure 5: **Fuel pellet outer radius with ENIGMA and eq. 1 and 2. In lower group of points coolant temperature is 20 ^{o}C and linear heat ratio =0**

With the default parameter values shown below, equation 3 gives very similar values for the hot fuel pellet radius as the equation 2.

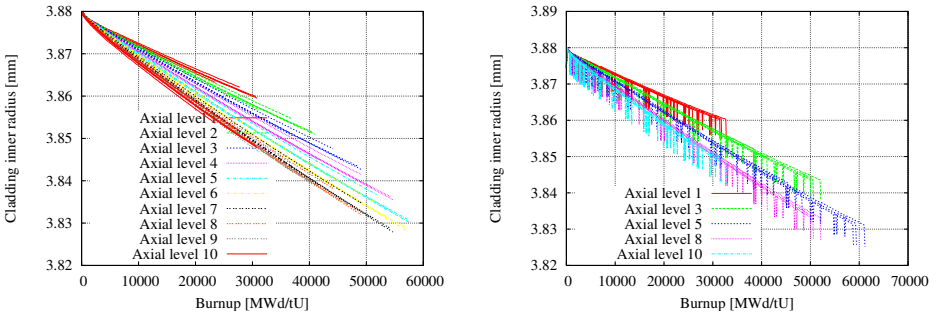
$$\alpha_1 = 8.55 \cdot 10^{-6}$$
$$\alpha_1 = 1.2793 \cdot 10^{-9}$$
$$\alpha_1 = 1.32 \cdot 10^{-12}$$

3.2 Cladding inner radius

When cold time steps were not included to the calculation, it seemed that inner radius of fuel cladding has a linear dependence on the burnup and slope depends linearly on the cladding temperature, Figure 6a. However, cold time steps revealed, that such assumption is not suitable. Instead, it seems that slope is dependent on the axial level, Figure 6b. So, instead of linear dependence of cladding temperature, temperature history of coolant was selected as an independent variable and dependence on the temperature was of the same exponential form as is in ENIGMA's secondary creep formulation:

$$R_{clad} \propto e^{c/T} \tag{4}$$

Cladding temperature would probably be more exact as a independent variable, but coolants temperature history is known quantity when initial state of the reactor dynamic calculation is determined. ENIGMA's creep parameter CRPC(5) defines rate of secondary creep and thus affects strongly to the cladding radius. Some test calculations were made with varied creep parameter, but curve was fit to the data in which creep parameter has the constant value.



(a) No cold time steps (b) Cold time steps included

Figure 6: **Cladding inside radius at different axial levels in five ENIGMA calculations.**

First trial was to fit the equation 5 to the data from different axial levels. However, it was find out that constant b decreases approximately linearly from lower to higher axial layers. Thus constant value b in equation 5 was replaced by term bT and finally equation 6 was fitted to the cladding outer radius values calculated by ENIGMA at the cold time steps.

$$R_{clad} = (1 + b + ae^{\frac{-c}{T_K}}Bu) \tag{5}$$

$$R_{clad} = R_0(1 + bT_K + ae^{\frac{-c}{T_K}}Bu) \tag{6}$$

Fitted curve and the cladding inner radius calculated with the ENIGMA at cold time steps are shown in Figure 7. Only some axial levels are shown to make curves readable. Value for the parameter c in equation 6 is same as creep correlation parameter CRPC(6) in ENIGMA input and R_0 is initial manufacture radius of cladding. Other parameter values for the equation 6 were:

$$a = -0.000119064$$
$$b = -1.818155 \cdot 10^{-6}$$

For the thermal expansion of cladding same model is used as in FRAPTRAN [6]:

$$R_{clad}(T_{K,clad}) = R_{clad}(T_{K,clad} = 293K)(1 - 1.485 \cdot 10^{-3} + 4.95 \cdot 10^{-6}T_{K,clad}) \tag{7}$$

Cladding inner radius calculated by ENIGMA and with the equations 7 and 6 are shown in Figure 8. Temperature $T_{K,clad}$ in equation 7 is average temperature of cladding and T_K in equation 6 average coolant history temperature. During the normal operation cladding and coolant temperature are near each other and thus thermal expansion of cladding is same although coolant temperature is used also in equation 7, as is done in figures of this report.

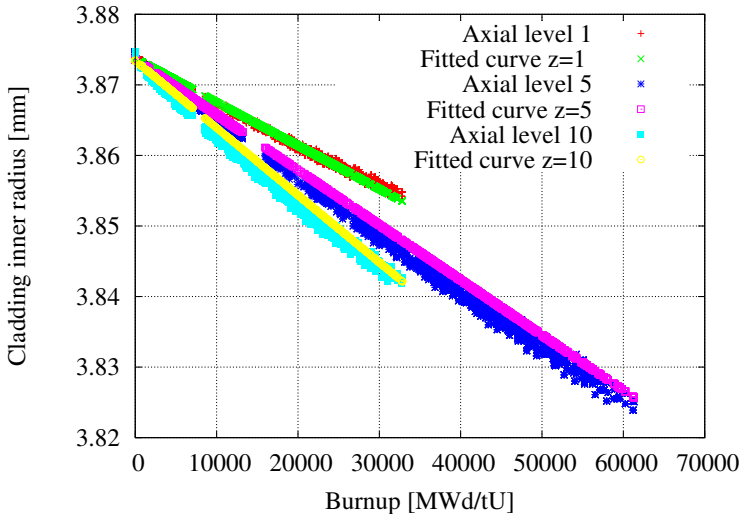


Figure 7: **Cladding inside radius at different axial levels calculated by ENIGMA and equation 6. Coolant temperature is 20 C and LHR=0**

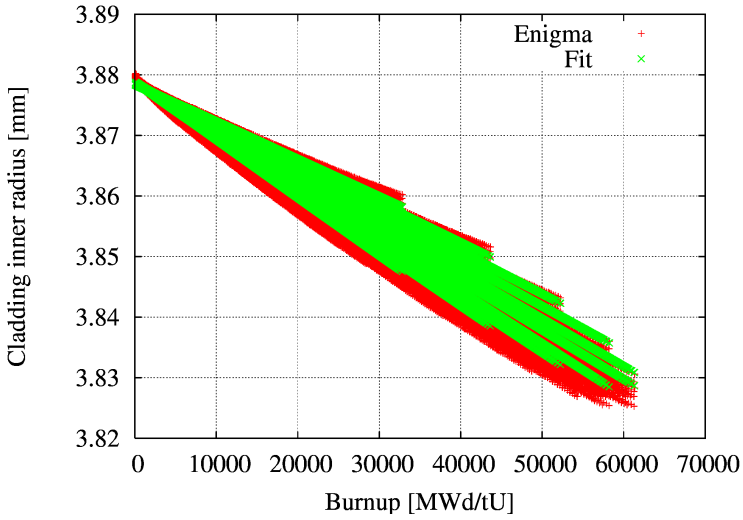


Figure 8: **Cladding inside radius at different axial levels calculated by ENIGMA and equation 7.**

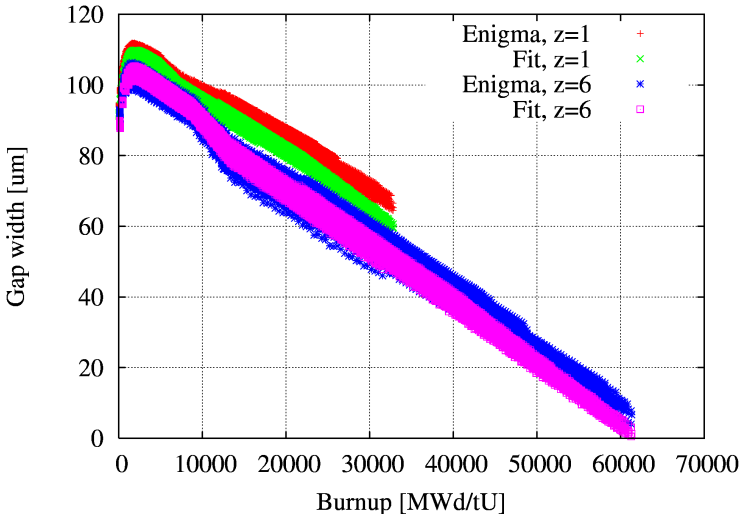


Figure 9: **Width of the gas gap at two different axial level with ENIGMA and with equations 7 and 1**

Approximation for the width of the gas gap can be shown in figure 9.

In these ENIGMA calculations only minor fission gas release was detected and gas gap remains open.

4 Utilization of data in reactor dynamic codes

The fuel performance codes are designed to assure safety of fuel rods in different kind of challenging situations, and thus it is important to consider several complicated phenomena with sufficient accuracy. In the reactor dynamic codes detailed description of fuel rods is not needed, but some features of fuel rod affect even on the behaviour of whole reactor. One of the most relevant, but in the same time inaccurately modelled feature is heat transfer in gas gap.

Several ways to model heat transfer have been implemented to the reactor dynamic codes HEXTRAN, TRAB-3D and TRAB. Most often value for the gas gap conductance is given in some temperature points and temporary value is interpolated from this given values. Typically own tables are given for fresh, one year old, two year old and three year old fuel. Same table is used for all assemblies and all axial levels, and only gas gap temperature has been changed from node to node. It is possible to interpolate also from two-dimensional table, where gas gap conductance is given as a function of temperature and burnup, but due to the deficiency of proper data this method has been used only in some occasional transient analysis calculation.

Correlation for gas gap conductance given in equation 8 has been implemented to all VTT's reactor dynamic codes [7], but it has been used at most in very early calculations with TRAB-1D and TRAWA.

$$h(T_g) = min\Big(h_{max}, \frac{1 + a_3 T_g + a_4 T_g^2}{a_1 + a_2 + T_g}\Big) \tag{8}$$

T_g in equation 8 is function of the surface and mean temperatures of the pellet.

Also possibility to give own temperature dependent curve for each node has been implemented, but tested only technically, not with a real nodewise data [8]. Some efforts have also been made to include models for the mechanical behaviour of fuel rod to the reactor dynamic codes [9]. However, this kind of approach was found too complicated, as long as VTT has not own fuel performance models and codes that could be utilized. Problem is also, that in the reactor dynamic calculations only some limited period of time has been modelled, starting from some predefined initial state. Properties of the fuel rod change all the time during its reactor life. These changes between the manufacturing and the initial state should also be modelled, not only the changes during the transient.

One possibility to utilize ENIGMA calculations in reactor dynamic codes is to give a gap width for a cold state as an input and model thermal expansion in the reactor dynamic code. With this method, also the changes during the transients could be modelled.

Changing dimensions of fuel rod may demand some modifications to the nodalization and data structures. One possibility is to use changing gas gap or "thermal gap width" width as an additional quantity, that is utilised only in heat transfer calculation.

4.1 Gas gap conductance

Gas gap conductance can be calculated with different kind of correlations, in which gas gap conductance depends on the gap width and gas composition. In these ENIGMA calculations only minor fission gas release happened. Thus fission gas composition was assumed to stay constant and include only Helium gas.

MATPRO correlation has been included to the TRAB-1D code in 1999 [9]. At that time intention was to model also dimensional changes inside the reactor dynamic codes. However, it was found out that geometry changes cannot be implemented to 3-dimensional reactor dynamic codes in such a simple way.

Gas gap conductance for the single gas is represented in MATPRO and FRAP-TRAN in similar way according to equation 9.

$$h = \frac{k}{t + x_{jump}} \tag{9}$$

In the equation 9 k is conductivity of gas and t width of the gas gap. x_{jump} is temperature jump distance that describes noncontinuum effects of heat transfer and becomes significant only with small gap widths. In the manual of MATPRO temperature jump distance of single gas is given with the equation 10. In the FRAPTRAN temperature jump distance is slightly different, eq. 11.

$$x_{jump,MATPRO} = \frac{4k}{(a_i P_i)\frac{(\gamma-1.)}{(\gamma+1.)}\sqrt{\frac{TM\pi}{2.R}}} \tag{10}$$

$$x_{jump,FRAPTRAN} = \frac{0.024688k\sqrt{1000T_{gas}}}{P_{gas}\sum \frac{f_j a_j}{\sqrt{M_j}}} \tag{11}$$

M in the equations 10 and 11 is molecular weight [kg/mole] of the gas and a_i accommodation coefficient if the gas. According to the MATPRO, accommodation coefficient for helium is:

$$a_{He} = 0.425 - 2.3 \cdot 10^{-4} T_{gas}$$

For the gas mixture equation 12 is given in MATPRO

$$h_{mix} = \sum_{i=1}^{n} \Big(\frac{k_i x_i}{x_i + \sum_{j=i\neq 1}^{n} \Psi_{ij} x_j} \Big) \Big(\frac{1}{t + \frac{\sqrt{M_i T}}{18}(\frac{\gamma_i - 1}{\gamma_i + 1})(\frac{1}{a_i P_i})(\frac{k_i}{x_i + \sum_{j=i}^{n} \delta_{ij} \Psi_{ij} x_j})} \Big) \tag{12}$$

If only Helium is present in gas gap, this equation gives different values than equations 9 and 10.

Gas thermal conductivity is calculated in FRAPTRAN with MATPRO model, equation 13.

$$k_i = A_i T_K B_i \tag{13}$$

Following parameter values were given for Helium

$$A_{He} = 2.639 \cdot 10^{-3} B_{He} = 0.7085$$

For the conductivity of gas mixture equation 14 is given.

$$k = \sum_{i}^{n} (\frac{k_i x_i}{x_i + \sum_{j=1}^{n} (1 - \delta_{ij}) \Psi_{ij} x_j}) \tag{14}$$

where

$$\Psi_{ij} = \phi_{ij} \big(1 + 2.41 \frac{(M_i - M_j)(M_i - 0.142 M_j)}{(M_i + M_j)^2} \big)$$

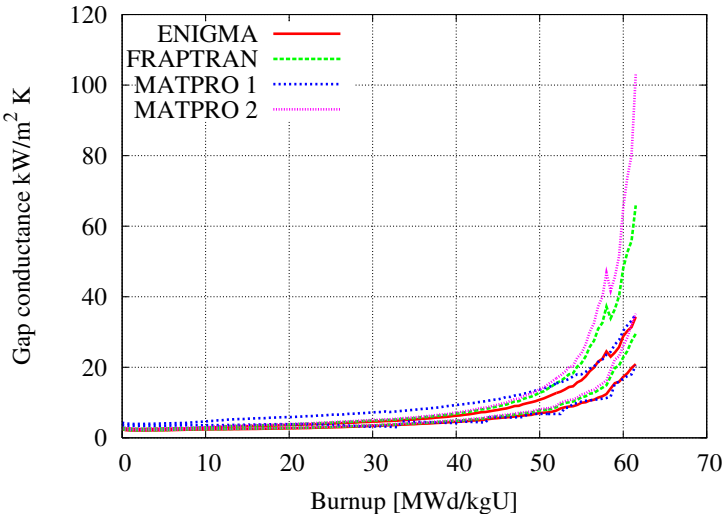


Figure 10: **Minimum and maximum value of gap conductance with different models. Width of the gas gap is calculated with equations 1 and 7 for MATPRO and FRAPTRAN models.**

and

$$\phi_{ij} = \frac{(1 + (\frac{k_i}{k_j})^{1/2}(\frac{M_i}{M_j})^{1/4})^2}{2^{3/2}(1 + \frac{M_i}{M_j})^{1/2}}$$

and

$$\delta_{ij} = \text{Kronecker Delta} = \begin{cases} 1 & \text{for } i = j, \\ 0 & \text{otherwise} \end{cases}$$

n = number of components in mixture
M_i = molecular weight of component i
x_i = mole fraction of the component i

In test calculations separate program was used for testing of different models. Burnup and temperatures calculated by ENIGMA was given as an input to test bench code. Gas gap conductance was calculated with different correlations and compared to the gas gap conductance calculated by ENIGMA in points. Results are shown in Figure 10, where minimum and maximum value of gap conductance are shown with different models. It can be seen that with high burnups FRAPTRAN, eq. 11 and MATPROmix, eq. 12 models give higher conductance than ENIGMA and MATPRO, eq. 10. With burnups 0-50 MWd/tU ENIGMA gives higher conductance values with some temperatures. Partly the difference with higher burnups can be explained by the fact that equations 1, 2 ,7 gives too small values for gap width compared to ENIGMA. However, there is difference also in conductance models, as can be seen from figure 11

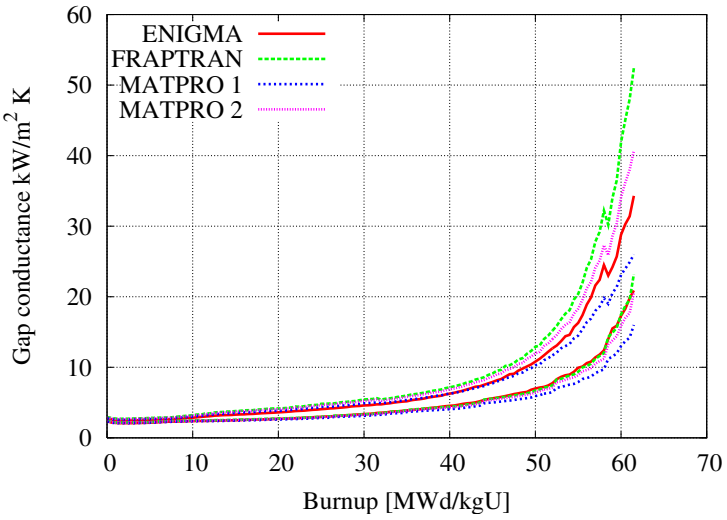


Figure 11: **Minimum and maximum value of gap conductance with different models, width of the gas gap is from the ENIGMA calculations.**

4.2 Conclusions

Aim of this work was to determine the properties of a representative rod at various points of its reactor life and thus enable an initialization of rod properties when no exact power history is known. Other aim was the updating of statistical version of the ENIGMA code and to introduce new person to nuclear fuel modelling.

Existing statistical ENIGMA did not include all newest updates of normal non-statistical ENIGMA. At the same time of starting this work, the normal ENIGMA was transferred to VTT's new linux cluster computer, which demanded some modifications to the code. Instead of updating the old statistical version of the ENIGMA code, new auxiliary script for performing statistical analysis was made. With the new script, it is always possible to use up-to-date version of the non-statistical ENIGMA also for the statistical calculations.

With the renewed statistical ENIGMA code, a VVER440 fuel rod was modelled by using artificial power history. Relationships between different characteristics were studied. As a result, width of the gas gap was chosen to be represented as a function of burnup. When curve fitting was made, it was find that also temperature dependence has to be included to the function. Fitting was made to the rods at the cold state and operation conditions were modelled by adding thermal expansion to the model. With this kind of model, also behaviour during the transient can be modelled, if data is utilized in the reactor dynamic codes.

As a result crude model for width of the gas was found. Several phenomena affecting to the rod are not modelled in physically proper way. However, the aim was to find some simple model that can be utilized in the reactor dynamic codes.

The model should be tested also with real power and temperature history. Also the whole procedure should be tested with different type of fuel assemblies.

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