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Comparing Different Approaches to Calculating Decay Heat Power of a Spent Fuel Dry Storage Cask for Krško NPP

Vid Merljak
Krško NPP
Vrbina 12, SI-8270 Krško, Slovenia
vid.merljak@ijs.si

Marjan Kromar
Jožef Stefan Institute
Jamova cesta 39
SI-1000 Ljubljana, Slovenia

ABSTRACT

One of the main limitations for dry storage of spent nuclear fuel is its decay heat power. Direct measurements are quite rare since they are time-consuming and expensive to perform. Therefore, computational approaches have been devised in the past to calculate the decay heat power. We can distinguish at least three approaches: 1) using (semi-)empiric formulae; 2) physics calculation while grouping fuel assemblies with similar characteristic and using only the most limiting value of each parameter (the so-called bounding approach); or 3) best-estimate calculation using explicit data of each fuel assembly.

In this paper, we compare results of such calculations for the proposed case of two limiting dry storage casks, each with 37 spent fuel assemblies from the Krško NPP. Best-estimate calculations were run with the ORIGAMI Automator (OA) of SCALE 6.2.2 code system, while the fuel assembly data was taken from an official Fuel Assembly Register (FAR) database. Due to data-intensive and error-prone input to OA project, a Python script interface FAR2OA was made and is briefly described here. Final results of decay heat power comparison are rather surprising – a considerable, 20 % relative deviation is found between the two calculation approaches. No clear explanation is found, however, initial checks are made and suggestions for further research are given.

1 INTRODUCTION

It is almost unnecessary to stress how the biggest difference of nuclear energy from other energy producing options is the existence of decay heat. The ability to correctly and (sufficiently but not over-) conservatively calculate the decay heat power (DH) of nuclear fuel assemblies (FAs) is therefore of utmost safety importance.

Several approaches have been developed to tackle this problem. A semi-empiric approach combines solving some physics-based equations for a certain FA history with interpolation of tabulated values that were obtained either from some generic calculation or from measurements. US NRC Regulatory Guide 3.54 [1] (hereinafter abbreviated as RG) provides a recipe for such approach. Here, detailed FA burnup history data is used. Because any single nuclear utility typically stores several hundred FAs, each with its unique burnup history, it is pragmatic to use the so-called bounding approach. With it, we get an upper bound of DH for several FAs at once – provided they can be bundled into groups with similar burnup characteristics. Nevertheless,

with faster computers, extensive digital data storage, and more and more computer program automation, it is nowadays feasible to calculate the DH explicitly for each particular FA. One such program for best-estimate calculations is ORIGAMI Automator (OA) of the SCALE 6.2.2 code system [2]. It solves the Bateman equations for more than two thousand nuclides. Reported numerical *precision* is better than 10^{-5}, therefore the *accuracy* of the whole calculation is nowadays governed by input nuclear cross-section libraries, underlying neutron transport accuracy, methodological assumptions, and quality of the input data.

The comparison in this paper is split into two parts. Firstly, since RG provides an example FA data with measured DH, it is reproduced in detail with both RG and OA, verifying our calculation approach. The second part of method comparison is the estimation of DH for two dry storage casks planned for Krško NPP Spent Fuel Dry Storage (SFDS) Campaign 1. Casks No. 8 and 14 were chosen because they have the highest and the lowest DH, respectively.

2 THEORETICAL BACKGROUND & COMPUTER PROGRAMS

As already mentioned, ORIGAMI Automator solves Bateman equations for more than two thousand nuclides. All results are stored in a binary file, so they can be viewed later on. This means that with only one calculation we can assess the DH of any combination of nuclides (as will later be used in Table 1). How the Bateman equations are actually solved numerically is beyond the scope of this paper and can be viewed in [2].

2.1 FAR2OA Script

Best-estimate calculations were run with the ORIGAMI Automator (OA) of SCALE 6.2.2 code system [2], while the fuel assembly data was taken from an official NPP Krško Fuel Assembly Register (FAR) database. Due to data-intensive and error-prone input to OA project, a Python script interface FAR2OA was made and is briefly described here.

FAR2OA is a Python module (package) designed to be run from command prompt. Given a Fuel Assembly Register (FAR) database exported to CSV format, it produces JSON files for all FAs detected, and arranges these files according to OA project sub-folder structure. Thorough testing of FAR2OA during the coding phase confirmed proper operation of core and advanced capabilities. That is, checking for any data anomalies, detection of FAs being currently irradiated in the reactor, duplicated lines and FA movement within spent fuel pool (SFP), initial material-accounting (e.g. handling of FA axial homogenisation), etc. are all handled automatically. Burnup achieved by any single FA in certain operational cycle is also calculated. Additionally, utility functions are provided. For example: to sort files by FA ID or to append operations entry (in our case the proposed FA insertion into dry storage cask at a certain Loading Date).

2.2 Regulatory Guide 3.54 (RG)

For the semi-empiric approach, the DH was calculated according to Rev.2 of the US NRC Reg. Guide 3.54, Spent Fuel Heat Generation in an Independent Spent Fuel Storage Installation [1] (RG). Decay heat power is split into five contributions,

$$P_T(t,T) = P_F(t,T) + P_C(t,T) + P_E(t,T) + P_A(t,T) + P_S(t,T)\,, \tag{1}$$

where index F denotes DH from *fission* product decay (excluding neutron capture), C from neutron *capture* to product ^{134}Cs, E from neutron capture on *other* fission products, A from *actinides*, and S from activated *structural* materials. Since contributions E and S are treated proportional to fission product decay term, P_F, and including a safety factor, F_S, the "safety-factor-corrected" DH can be written as

$$P'_T(t,T) = F_S \times [[1 + H(t) + A(t)] \times P_F(t,T) + P_C(t,T) + P_A(t,T)] \,. \quad (2)$$

Note that RG Rev.2 [1] is relatively new (published in 2018). Before that, Rev.1 [3] did not cover high burnup fuel, which was the reason for publishing special document [4] that provided temporary guidelines for treating such FAs. Differences to previous revision are briefly discussed in Appendix A of [1] and are not treated here. In essence, Rev.2 extends the applicability ranges and "reasonably reduces" the conservativism margin.

2.3 Safety Factors

The safety factors (F_S), aimed at providing a sufficient DH margin to cover for possible calculation or operational outliers, can be assigned in various ways. RG [1] employs tabulated F_S, ranging from 1.02 (2 % addition) for less than 10^9 seconds (≈ 31.7 years), and rising up to 1.06 for approx. 127 years since last irradiation. Krško NPP sub-contractor for the SFDS project used the following linear function:

$$P'_T(t,T) = P_T(t,T) \times (1 + 10\ \%) + a(t) \,, \quad (3)$$

where $a(t)$ depends on the time/date of reporting: 81 W for loading date and 31 W for transport date (which is 7 years later). This approach introduces a significant bias for low DH fuel assemblies. This is not very useful for comparing different approaches to calculate the DH. It is, however, practical when trying to conservatively asses the dry storage casks thermal load. To ensure an equal basis, we compare values without safety factors. Any deviation from this rule is annotated appropriately.

3 RESULTS

3.1 Reference Case

It is interesting to compare OA with RG example (Table 1) because reference *measured* DH is provided. Since the OA results do not include any safety factor, we also display RG result without it (e.g. $F_S = 1$ instead of 1.02). Additionally, partial contributions from ^{134}Cs and seven major actinides (according to [1]) are given for RG and OA.

Table 1: Decay heat power for the fuel assembly C-64 example.

	Measured (from [1])	RG (Rev.1) $F_S = 1$	RG (Rev.1) $F_S = 1.0724$	RG (Rev.2) $F_S = 1$	RG (Rev.2) $F_S = 1.02$	OA (our work)
DH [W]	931.0	950.8	1019.6	960.4	979.6	907.7
Rel. Dev.	(Ref.)	+2.1 %	+9.5 %	+3.2 %	+5.2 %	-2.5 %
P_C [W]	/	/	/	169.1	/	165.9
P_A [W]	/	/	/	144.5	/	130.2

We see that calculated values without safety factors lie in ±3 % interval of measured DH value and that Origami Automator is the only one that predicts *lower* DH value than measured (i.e. non-conservative value). This will be important for interpreting other results. It may also be noted that OA under-predicts the DH of both P_C and P_A contributions. This makes it less likely that an error or deviation originates in only one of the DH partial contribution terms.

3.2 Krško NPP Proposed Dry Storage Casks

The FA-wise results for dry storage Cask No. 8 are summarised in Table 2. Although Cask 8 has the highest DH and Cask 14 the lowest DH, relative deviation between OA and RG is very similar in both cases. Due to lack of space, FA-wise results for Cask 14 are therefore not given in detail. Integral values of DH for both casks are given in Table 3, while Figure 1 displays all DH data at Loading Date.

Table 2: Decay heat power for Cask No. 8 at cask Loading Date.

FAID	Days since 1st irradiation	RG (Rev.2) $F_S = 1$	OA (our work)	Relative deviation
HH11	11436	717	583	-18.7 %
K25	10641	609	484	-20.5 %
L03	9534	621	510	-17.9 %
N13	9029	664	528	-20.5 %
P13	8613	801	621	-22.4 %
P21	8613	659	515	-21.8 %
P23	8613	658	515	-21.7 %
P27	8613	652	511	-21.7 %
R16	8289	589	471	-19.9 %
S11	7936	735	577	-21.5 %
S26	7582	619	502	-19.0 %
T05	7582	693	544	-21.5 %
T07	7582	676	532	-21.3 %
T17	7582	691	542	-21.5 %
T20	7582	675	532	-21.3 %
T25	7582	698	548	-21.5 %
T26	7582	747	588	-21.3v%
U28	7188	695	547	-21.3 %
V16	6821	812	634	-22.0 %
V27	6821	815	636	-22.0 %
V28	6821	810	632	-22.0 %
X27	6104	744	585	-21.4 %
X44	6104	822	641	-22.0 %
Y05	5618	844	665	-21.3 %
Y29	5618	954	749	-21.5 %
Y41	5618	957	752	-21.5 %
Y51	5618	953	748	-21.5 %
AA28	5033	693	563	-18.8 %
AB40	4488	975	776	-20.5 %
AC31	3945	1239	987	-20.3 %
AC32	3945	1238	986	-20.3 %
AC47	3945	1039	838	-19.3 %
AC48	3945	1041	840	-19.3 %
AC49	3945	1033	833	-19.3 %
AC51	3945	1044	842	-19.3 %
AC55	3945	1071	864	-19.4 %
AD04	3398	1092	901	-17.4 %

Table 2 (continued): Decay heat power for Cask No. 8 at cask Loading Date.

	Days since 1st irradiation	RG (Rev.2) $F_S = 1$	OA (our work)	Relative deviation
RMSE	/	/	/	20.7%
MEDIAN	/	/	/	-21.3%
SUM	/	30377	24121	-20.6%

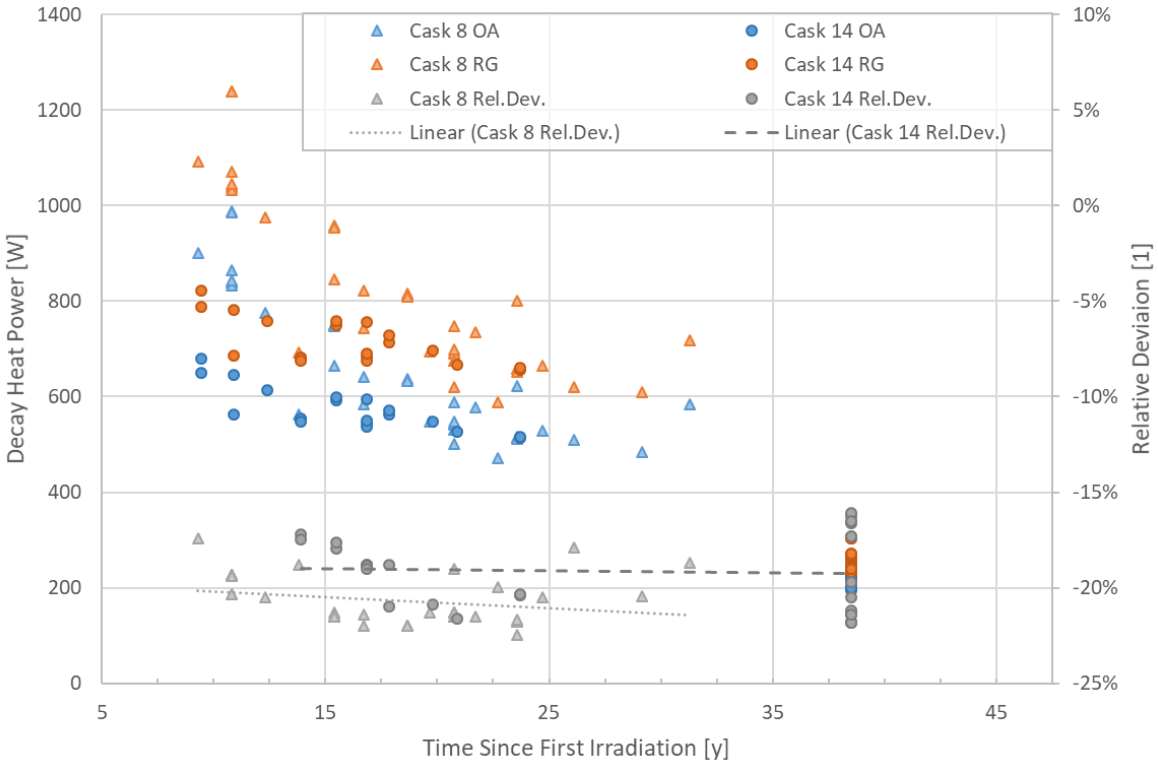

Figure 1: DH comparison for Casks 8 and 14 at Loading Date. Analogous figure for the Transport Date is very similar and is therefore not displayed.

Table 3: DH for Casks No. 8 and 14. Transport Date is 7 years later than the Loading Date.

	Loading Date			Transport Date		
Cask	RG (Rev.2) $F_S = 1$	OA (our work)	Rel. dev.	RG (Rev.2) $F_S = 1$	OA (our work)	Rel. dev.
8	30377	24121	-20.6 %	25822	20081	-22.2 %
14	19044	15413	-19.1 %	16517	13147	-20.4 %
SUM	49421	39534	-20.0 %	42339	33228	-21.5 %

Surprisingly, the relative deviation lies around minus 20 %! I.e. not employing any kind of safety factors, the DH values calculated by the ORIGAMI Automator are significantly lower than the values obtained following the RG procedure. Naturally, there are (at least) two sides to this. After satisfactorily ruling-out possible input errors, options are that either the OA gives unrealistically low values or RG employs excessive conservativisms in some of its sub-steps. Which of these options holds true remains to be determined. As Figure 1 shows, relative deviation between OA and RG is almost unaffected by the time since first irradiation (i.e. the age of FAs). It is possible that some other systematic effect or error is in place.

3.3 Discussion

One point, where the RG calculation could be challenged is that about a quarter of all FAs fall outside the applicability range for specific power (i.e. from 12 kW/kgU to 50 kW/kgU). FAs from fuel region AA onwards may deplete in their first operating cycle with specific power up to 55 kW/kgU. This is 10 % above the upper limit. Nevertheless, deviation between RG and OA for these FAs does not differ from deviation for other FAs, which dispels this as a possible explanation.

In OA, the user can define an arbitrary and fuel-cycle-dependent *shape* of the cycle power profile. In RG, the assumed profile is constant specific power throughout each of the cycles, only varying in their intensity. Switching from single-step to three-step power history in OA changes the resulting DH by less than 0.1 %.

Another possible explanation for the observed DH deviation could lie in some error in the used computing tools. Therefore, the RG reference case from Subsection 3.1 was recalculated with SCALE versions 6.2.3 and 6.2.4. The resulting DH was 900.2 W and 907.7 W, respectively. (The latter is completely identical to what we obtained with version 6.2.2.) Simply using different versions of the same code changed the DH by about 1 % – clearly less than the 20 % we are trying to explain.

Just recently, Čalič and Kromar researched how various nuclear data libraries impact the spent FAs' characteristics [5]. They found that DH is affected by no more than 2.5 %. Furthermore, differences peaked at two particular cooling times – 0.1 years and 100 years – whereas in-between (say at 4.5 years cooling time as in our RG reference case) they dropped to a local minimum of only −0.5 %. Mind that research from [5] pertains to the same fuel design as in our aforementioned Krško NPP SFDS case.

And perhaps this could actually be the most notable difference of our OA calculations from the RG results. Namely, the RG semi-empiric approach methodology is based, verified, and tuned to the prevailing 17×17 fuel design. In our best-estimate approach with OA, however, we explicitly modelled the fuel utilised in Krško NPP, i.e. the Westinghouse 16×16 fuel design. (For the reference case we used the W14×14 fuel design as described in RG [1], of course). RG states that different fuel designs influence the DH *to a minor extent* ([1] page 19), but nevertheless, to resolve this suspicion we propose that an analogous comparison be made with real W17×17 fuel history data.

Lastly, and in spite of objection listed in Subsection 2.3, we can check the DH deviation with safety factors taken into account. In Table 4, raw OA results were multiplied (FA-wise, of course) according to Equation (3).

Table 4: DH with safety factors.

	Loading Date			Transport Date		
Cask	RG (Rev.2, with F_S)	OA (with F_S)	Rel. dev.	RG (Rev.2, with F_S)	OA (with F_S)	Rel. dev.
8	30985	29530	-4.7 %	26339	23236	-11.8 %
14	19429	19951	+2.7 %	16860	15609	-7.4 %
SUM	50414	49481	-1.9 %	43199	38845	-10.1 %

While for the Loading Date the relative deviation is now within ± 5 %, it nevertheless gets worse than −10 % for the Transport Date. Also, it is clearly visible that for lower DH assemblies (Cask 14), adding a constant decay heat value (parameter $a(t)$) skews the comparison more than for high DH assemblies. Using safety factors to artificially make discrepancies look smaller is *not* a recommended way to go.

4 CONCLUSION

Overall, we have found that the two approaches considered for calculating the decay heat of spent nuclear fuel assemblies nowadays still yield considerably different values. In our Krško NPP case of two proposed casks for spent fuel dry storage, each filled with 37 fuel assemblies, both the relative deviation and RMSE differences were as much as (minus) 20 %. Clear explanation for deviation of such magnitude is yet to be identified. As for now, we can exclude the possibility of an input error and of some most obvious physics errors. It seems most likely, though, that the source of discrepancies lies in the non-common W16×16 fuel design used in the Krško NPP, which is not covered by the RG approach.

For further research we suggest making a backwards comparison to first revision of Regulatory Guide 3.54 [3] (along with its expansion of ref. [4]), and comparison to some other computer code for nuclear fuel depletion calculations. Also, an analogous comparison as in the present research, but on some benchmark W17×17 fuel history data is desirable.

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