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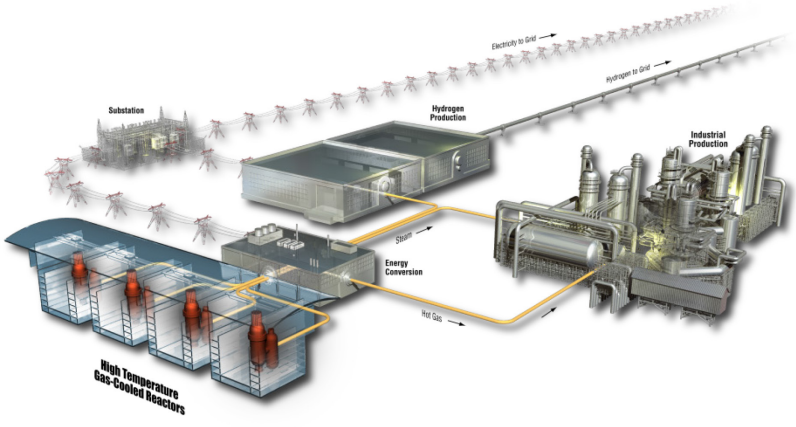
Revision 0

Decay Heat Quantification in the High-Temperature Test Reactor

Andrew Hummel and Sonat Sen

May 2017



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INL ART TDO Program

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ABSTRACT

The proper calculation of decay heat is necessary for both postulated accidents and normal spent fuel repository safety analysis. Since the 1970s, the nuclear industry has primarily relied on use of the American National Standards Institute (ANSI)/American Nuclear Society (ANS)-5.1 standard or one of its predecessors as the tool for calculating this heat. However, different reactor systems can have substantially different materials, neutron spectrums, operating characteristics, and so forth that lead to vastly different isotopic compositions in the fuel over time. The ANSI/ANS-5.1 standard is specific to light water reactors; therefore it may not be well suited for other systems such as high-temperature gas reactors.

Recent developments in the SCALE 6 code developed at Oak Ridge National Laboratory have allowed for a more accurate treatment of the complexity associated with high-temperature reactor tristructural isotropic fuel. Also, the isotopic depletion and generation code ORIGEN-S, now a module of SCALE, has been validated against experimental data for light water reactors for properly characterizing decay heat. And, most recently, Japan Atomic Energy Agency has used the ORIGEN code to generate high-temperature gas reactor cross-section libraries to be used to quantify the decay heat generated in the High-Temperature Engineering Test Reactor at the Oarai Research and Development Center. Given Idaho National Laboratory's continued research into the viability of high-temperature gas reactors as a next generation power reactor, an independent decay heat quantification analysis has been performed for a variety of fuel enrichments, tristructural isotropic particle packing fractions, and fuel temperatures using a similar approach. These data are then used as input into the RAVEN code developed at Idaho National Laboratory. A Reduced Order Model mathematical model in RAVEN is 'trained' to create a response mechanism to the various input parameters, which can later be used to predict the decay heat at a given time as a function of input parameters. Preliminary results demonstrate the potential for using this methodology to accurately predict decay heat generation.

CONTENTS

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ACRONYMS

ANS	American Nuclear Society
ANSI	American Nuclear Standards Institute
BP	burnable poison
FP	fission products
HTTR	high-temperature test reactor
INL	Idaho National Laboratory
JAEA	Japan Atomic Energy Agency
MA	minor actinides
RAVEN	reactor analysis and virtual control environment
ROM	reduced order model
TRISO	tristructural isotropic

Decay Heat Quantification in the High-Temperature Test Reactor

1. INTRODUCTION

1.1 Background

The proper calculation of decay heat is necessary for both postulated accidents and normally discharged spent nuclear fuel safety analysis. A first draft standard was issued by the American Nuclear Society (ANS) in 1971 [1] after numerous independent studies had already been conducted, most notably by Shure [2,3]. This standard has been used for light water reactors over the years and was updated in 1994 and again in 2005 to its current form, the American Nuclear Standards Institute (ANSI)/ANS-5.1-2005 standard [4]. This standard assumes ^{235}U is the major fissile material and contributions from ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu are each treated explicitly (^{239}Np and ^{239}U are also included). Decay heat generated from delayed neutron-induced fission, activation products in structural materials, and other actinides is not included in the ANSI model.

Because different reactor systems can have substantially different materials, neutron spectrums, operating characteristics, and so forth, isotopic composition in the fuel can vary widely from one system to another. The ANSI/ANS-5.1 standard is specific to light water reactors and might not be well suited for high-temperature gas reactors. Thus a comparative study was done by the Japan Atomic Energy Agency (JAEA) using the ORIGEN code to quantify the decay heat generated in the High-Temperature Engineering Test Reactor at the Oarai Research and Development Center [5]. ORIGEN is a summation code (i.e., integral quantities are determined by summing the individual contributions of radionuclides) that has been extensively used and benchmarked to accurately calculate isotopic changes over time, with its accuracy limited to the inherent accuracy and completeness of that of nuclear data itself [6,7]. The JAEA results were compared to the results from using both the ANSI standard and the Shure Equation, with relatively good agreement. Current research at Idaho National Laboratory (INL) has prompted an independent analysis into decay heat generation and behavior for the High-Temperature Test Reactor (HTTR) at a variety of fuel enrichments, fuel temperatures, and tristructural isotropic (TRISO) fuel packing fractions. These variables, along with the generated decay heat, are used as input into the Reactor Analysis and Virtual control Environment (RAVEN) [8] code developed at INL to yield a response function. This function can then be used in other transient analysis codes for predicting the decay heat based on the initial conditions. Preliminary results show this to be a very promising technique.

1.2 Methodology

The most accurate and robust methods for solving the neutron transport equation are those based on the Monte Carlo method. Although solutions are always mere approximations, this method allows for a continuous treatment of energy, no angular or spatial discretization, and very detailed three-dimensional geometrical representations. However, the results are statistics based and the computational time required to achieve meaningful results (i.e., those with low uncertainties) can be unpractical for many applications. The JAEA analysis [5] uses the Monte Carlo code, MVP, to yield reaction rates that are used in conjunction with the depletion code, BURN, which, in turn, calculates burnup-dependent isotopic compositions. However, the geometrical model used is a single HTTR pin cell. The analysis described in this document focuses on a typical fuel assembly lattice of the HTTR, which is a much larger and more detailed model than a pin cell. Coupled with the number of variables examined, using a Monte Carlo code did not seem like an appropriate option; therefore, a two dimensional lattice physics approach with only the SCALE package is used for all neutronic calculations.

1.2.1 Lattice Physics Calculation with SCALE

The SCALE package developed at Oak Ridge National Laboratory is a very versatile lattice physics code consisting of a multitude of different modules that can be coupled together with coordination of the control module, TRITON. The main calculation flow for this work is as follows: the module produce multi-group cross-sections (PMC) computes multi-group cross sections using the pointwise neutron spectra generated from the continuous energy treatment module [9]. This leads to problem-specific, self-shielded, multi-group cross sections in the doubly heterogeneous material. (Recent developments in the SCALE 6 version have allowed for a more accurate treatment of the complexity associated with the double heterogeneity of high-temperature reactor TRISO fuel compacts [10,11,12]). TRITON then passes these cross sections to the discrete-ordinates neutron transport solver (i.e., new extended step characteristic-based weighting transport code). NEWT uses the extended step characteristic approach to mesh the problem over arbitrary polygons and then performs a k-eigenvalue calculation. Upon completion, TRITON passes data to the depletion module ORIGEN, which solves the Bateman equations to obtain burnup dependent isotopics. These new isotopics then become the starting point to repeat the process until the final desired burnup is reached.

For each ORIGEN depletion calculation, the cross-section libraries (per user specified isotopes) are stored at each burnup state point. Once the simulation runs to completion, all state points are combined into one (.f33) file. The above procedure was carried out for each combination of fuel enrichment, fuel temperature, and TRISO packing fraction to obtain HTTR-specific cross-section libraries over a variety of operating parameters. (It should be noted that since the total block power is kept constant and not used as a parameter at this stage of the analysis, as the packing fraction changes, the cycle-specific power will change accordingly). The lower and upper enrichments were chosen because they represent the lower and upper bounds of that used in HTTR (i.e., 5.9% is the average). The different packing fractions represent a reasonable band around the average of 0.30. The nominal operating temperature is around 900K and additional temperatures cover the range of likely transients. The different parameters are given in Table 1, along with the appropriate specific power. Per the SCALE 6.2 user's manual, these libraries were added to the arplibs directory and the arpdata.txt file was updated accordingly. These libraries can now be interpolated with the ARP module and used directly by ORIGEN to determine the decay heat over a range of the three parameters. By varying these parameters, the decay heat can be generated at many different state points. The combination of every parameter at each different state point is then used as input for the RAVEN software tool, which is currently under development at INL, to perform a parametric evaluation.

Table 1. Parameters for generating HTTR-specific cross-section libraries.

Temperature (K)	Enrichment (^{235}U wt.%)	Packing Fraction	Specific Power (MW/t)
300	3.4	0.25	40.0
600	5.9	0.30	33.3
900	7.2	0.35	28.57
1200	9.9	0.40	25.0

1.2.2 Decay Heat-Reduced Order Model with RAVEN

RAVEN is a software framework able to perform parametric and stochastic analysis based on the response of complex system codes. Initial development was aimed at providing dynamic risk analysis capabilities to the thermohydraulic code RELAP-7, which is currently under development at INL. Although the initial goal has been fully accomplished, RAVEN is now a multi-purpose stochastic and uncertainty quantification platform that is capable of communicating with any system code. RAVEN is capable of investigating system responses and explores input space using various sampling schemes

(e.g., Monte Carlo, grid, or Latin hypercube). However, the strength of RAVEN lies in its system feature discovery capabilities (e.g., constructing limit surfaces, separating regions of the input space that lead to system failure, and using dynamic supervised learning techniques).

In RAVEN, models are important entities. A model is an object that employs a mathematical representation of a phenomenon, either of a physical or other nature (e.g., statistical operators). From a practical point of view, it can be seen as a "black box" that, given an input, returns an output. A reduced order model (ROM) is a mathematical model consisting of a fast solution of a physical system trained to predict a response of interest. The "training" process is performed by sampling the response of a physical model with respect to variations in its parameters subject (e.g., probabilistic behavior). The results (i.e., outcomes of the physical model) of sampling are fed into the algorithm representing the ROM that tunes itself to replicate those results. RAVEN supports several different types of ROMs, both internally developed and imported through an external library called "scikit-learn" [13]. The use of RAVEN in order to create ROM of the decay heat is shown in Section 2.2.

1.3 Model Description

A two-dimensional model of an HTTR assembly was built for this analysis. Some assemblies contain 33 pins, but the 31-pin assembly is more prevalent in the core and thus chosen for this work. As shown in Figure 1, the fuel (red) is annular in shape and consists of TRISO particles embedded in a graphite matrix with a 5.15-cm pitch. Helium gas flows inside the fuel compacts. There are two burnable poison (BP) channels (purple) in the corners of the assembly containing B4C, 2.0 wt.% 10B, and there is one helium channel (white) (in the southwest corner of Figure 1). The assembly matrix is graphite (green). The number densities for all fuel enrichments and BP are given in Table 2 and come directly from those used in the most recent International Criticality Safety Benchmark Evaluation Project report on HTTR [14]. Table 3 has all relevant dimensions. A total of 64 models ($4 \times 4 \times 4$) were depleted to various burnup levels depending on the appropriate specific power to generate the necessary HTTR libraries.

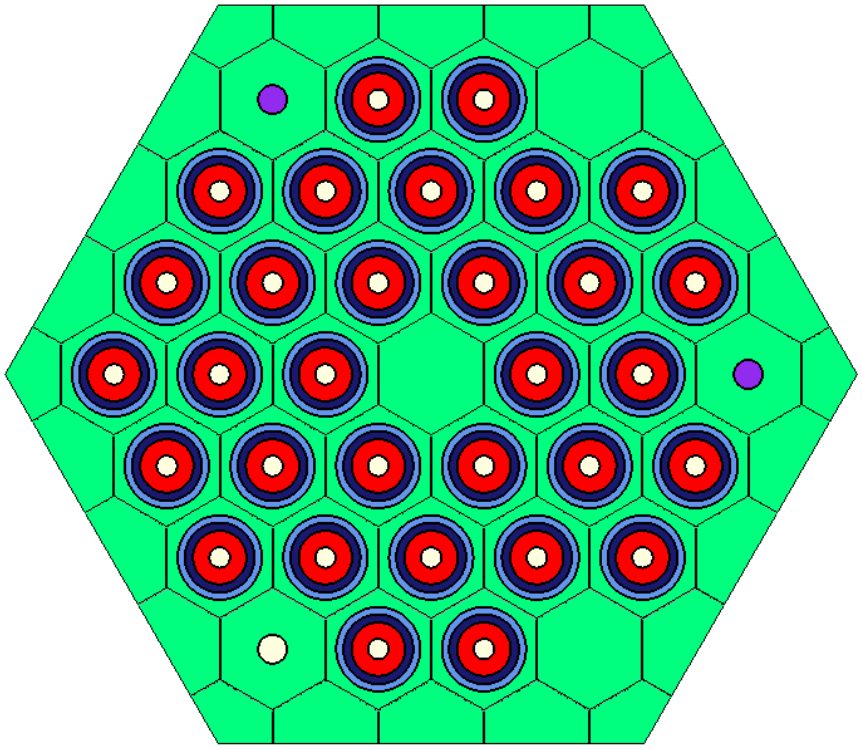

Figure 1. Two-dimensional model of a 31-pin HTTR assembly.

Table 2. Fuel and burnable poison number densities.

Material	^{234}U	^{235}U	^{238}U	O	^{10}B	^{11}B	C
3.4% fuel	6.1026E-06	7.9888E-04	2.2405E-02	4.6404E-02	1.7299E-07	—	—
5.9% fuel	1.0590E-05	1.3863E-03	2.1821E-02	4.6404E-02	1.7299E-07	—	—
7.2% fuel	1.2923E-05	1.6918E-03	2.1517E-02	4.6404E-02	1.7299E-07	—	—
9.9% fuel	1.7769E-05	2.3262E-03	2.0886E-02	4.6404E-02	1.7299E-07	—	—
2.0% BP	—	—	—	—	3.9906E-04	1.6063E-03	8.8446E-02

Table 3. Assembly geometry specifications.

Dimension	Length (cm)
Block side length	20.78461
Block apothem	18.0
Flat-to-flat	36.0
Pitch	5.15
Fuel pin radius	2.05
Fuel compact inner/outer radius	0.5/1.3
TRISO-coated fuel particle radii	0.03/0.036/0.039/0.0415/0.046
BP pin radius	0.7
Helium channel radius	0.75

2. RESULTS

2.1 Core Eigenvalue Dependency

The infinite multiplication factor changes over time as both the fuel and the BPs burn out. Figure 2 show the infinite eigenvalue as a function of burnup as the TRISO particle packing fraction changes from 0.25 to 0.40. The fuel temperature is 1200K and enrichment is constant at 5.9% (the average). Figure 3 presents the eigenvalue as the fuel temperature changes with a constant packing fraction and enrichment, and Figure 4 shows the eigenvalue as the enrichment changes. The effect of BPs on the excess reactivity over time can be seen in these figures; initially the excess reactivity is reduced and the k-infinity curve remains relatively flat for a time while the BPs and fuel burn out. The fuel enrichment values 3.4%, 5.9%, and 9.9% were chosen because they represent the least enriched pellets, the average pellet enrichment (i.e., the enrichment JAEA used), and the highest enrichment. The additional value of 7.2% was chosen to provide a more robust basis set of cross sections for interpolation.

For a given packing fraction, the higher the fuel temperature, the lower the core reactivity. This is expected due to Doppler broadening in the fuel. Also, as expected, the lower the fuel enrichment, the lower the core reactivity.

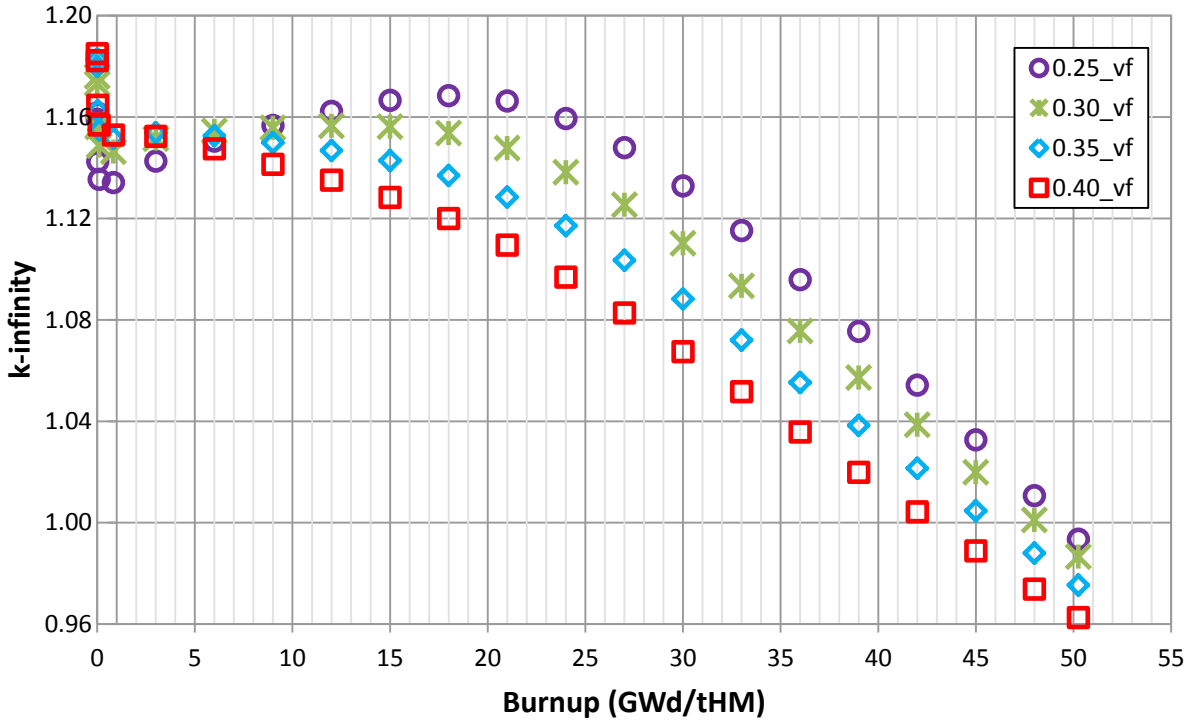

Figure 2. k-infinity as a function of packing fraction for 5.9% enriched fuel at 1200K.

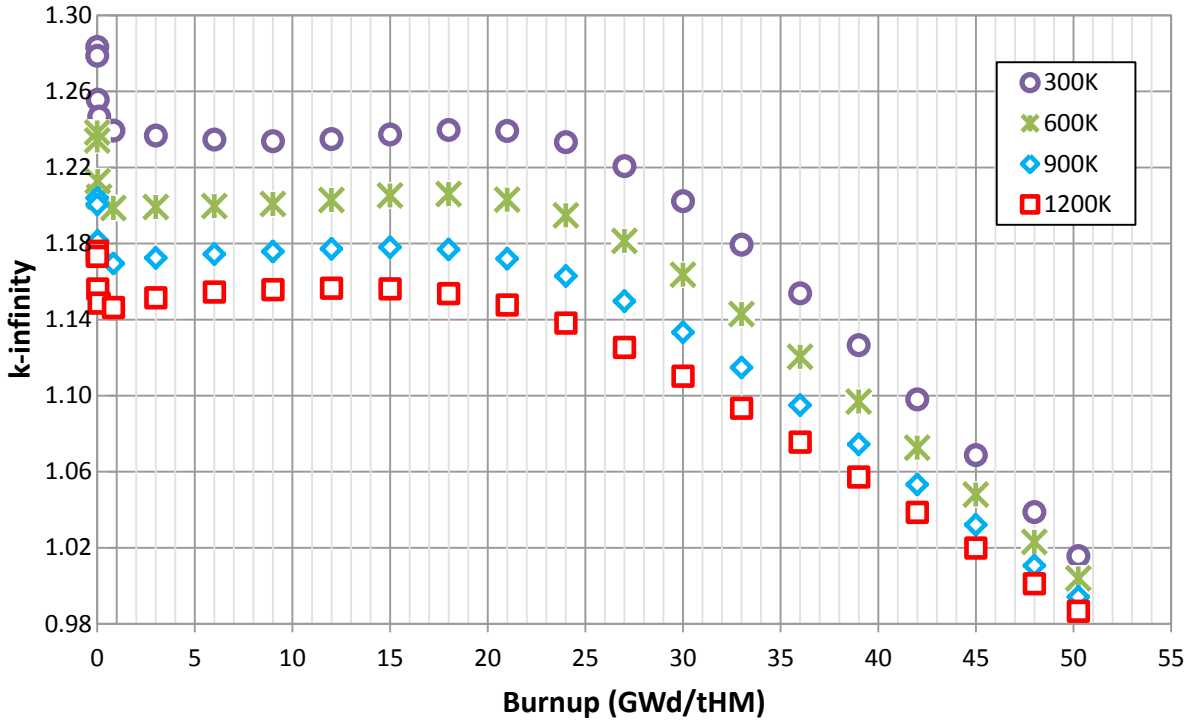

Figure 3. k-infinity as a function of fuel temperature for 5.9% enriched fuel and 0.30 volume fraction.

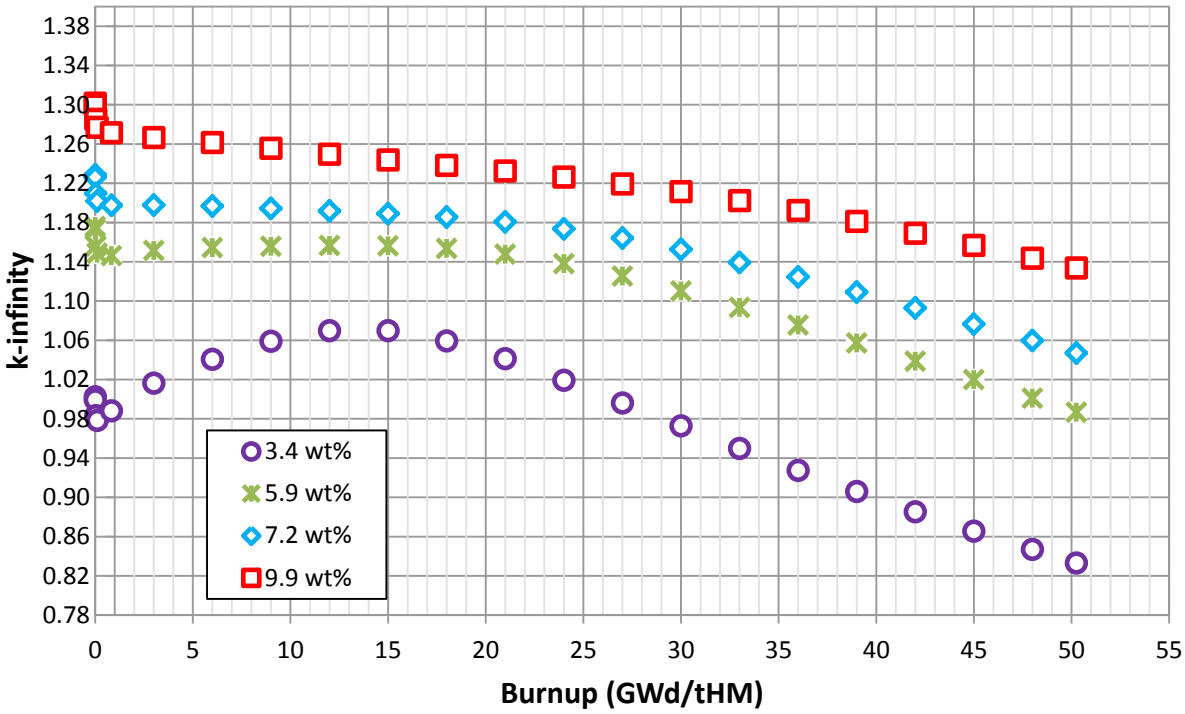

Figure 4. k-infinity as a function of fuel enrichment for a constant packing fraction of 0.30 and fuel temperature of 1200K.

2.2 Decay Heat Using ORIGEN

To compare the results to that of JAEA, the decay heat was calculated for 5.9% enriched fuel at 1200K with an average burnup of 22 GWd/t over 660 days. Figure 5, Figure 6, Figure 7 and Figure 8 show the decay heat for cooling times of 30 days and 5 years, respectively. The results clearly show that changing the TRISO packing fraction (with a corresponding change in specific power) has a direct effect on the amount of decay heat generated. After 30 days of cooling, decay heat is between 35 and 60 kW; after 4 years of cooling, decay heat is below 2.0 kW. Although the data points of the JAEA study [5] are not available, the graphs appear to be very comparable when examining the case with the same enrichment and volume fraction. Figure 9 shows how fractional contribution to decay heat from minor actinides (MAs) and fission products (FPs) changes as enrichment varies. As enrichment increases, the initial contribution to decay heat from MAs also increases. At 5.9%-enriched TRISO particles, decay heat due to FPs begins to dominate after approximately 80 years of cooling time. At a higher enrichment of 9.9%, the MA contribution remains dominant for a nearly 50% longer time period and is not surpassed by FPs until roughly 120 years of cooling time. Table 4 and Table 5 list the major isotopes that contribute to decay heat as a ratio for FPs and MAs when cooling time increases. The agreement with JAEA is especially good for FPs. On the other hand, some MAs (e.g., the Pu isotopes and ^{244}Cm) do not show particularly good agreement. However, it should be noted that the two different pin cell models used by JAEA also do not show good agreement with these same MAs (i.e., JAEA's two models have the contribution due to ^{244}Cm differing by nearly 44%). The JAEA results for the AC pin cell are included in Table 4 and Table 5 for comparison at 10 days and 5 years.

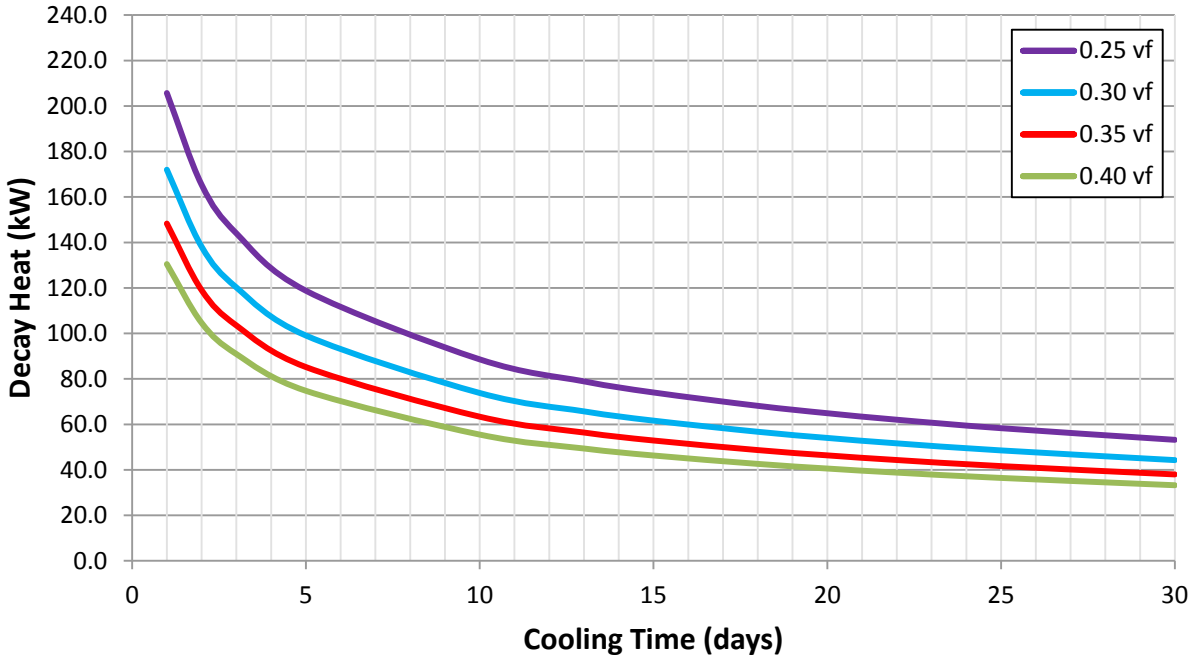

Figure 5. Decay heat generated over 30 days cooling for different packing fractions.

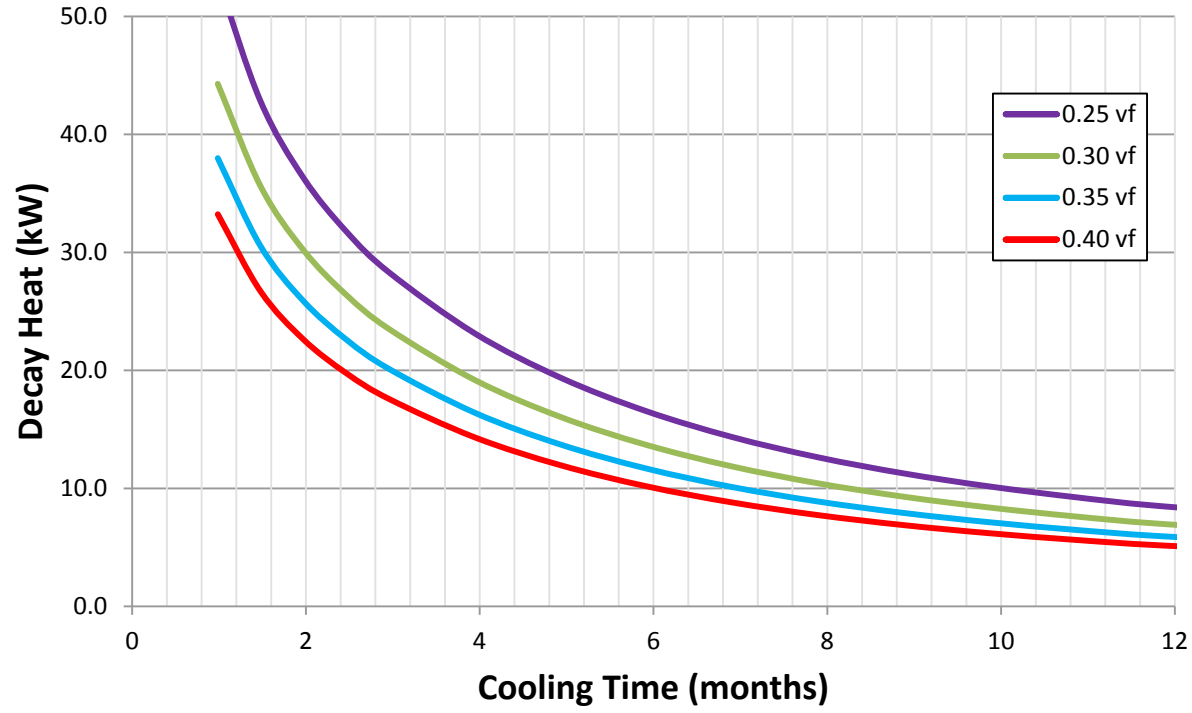

Figure 6. Decay heat generated over 12 month cooling for different packing fractions.

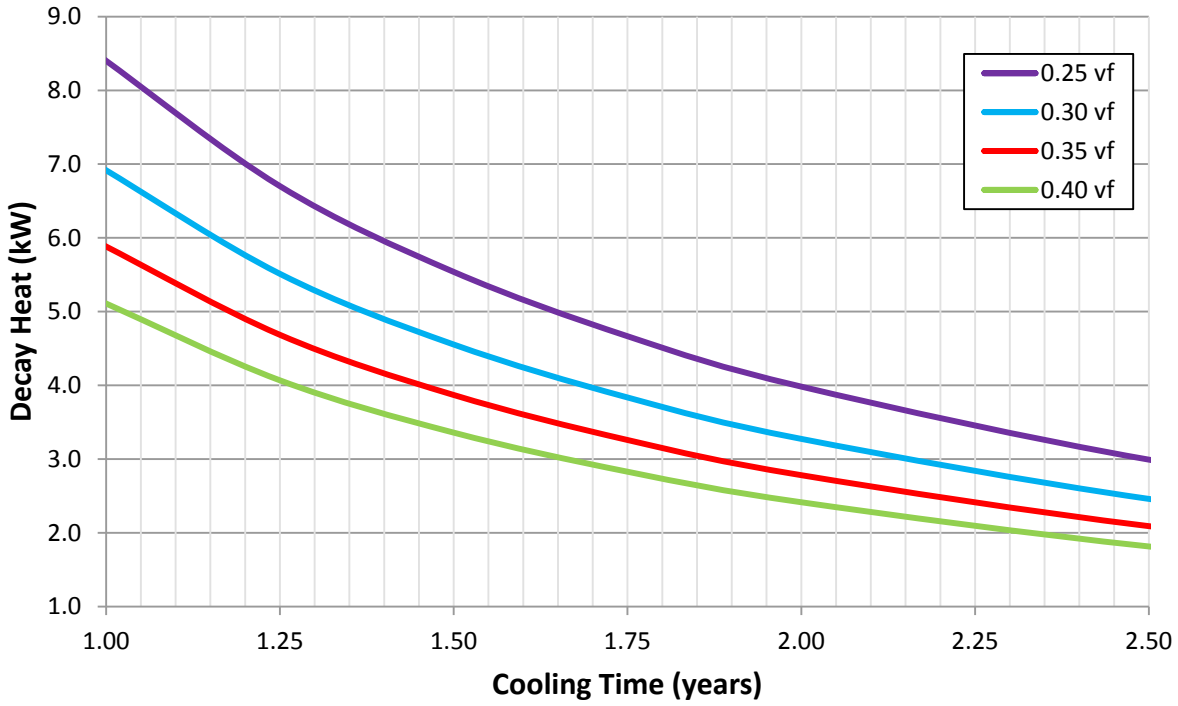

Figure 7.Decay heat generated between 1 and 2.5 years cooling for different packing fractions.

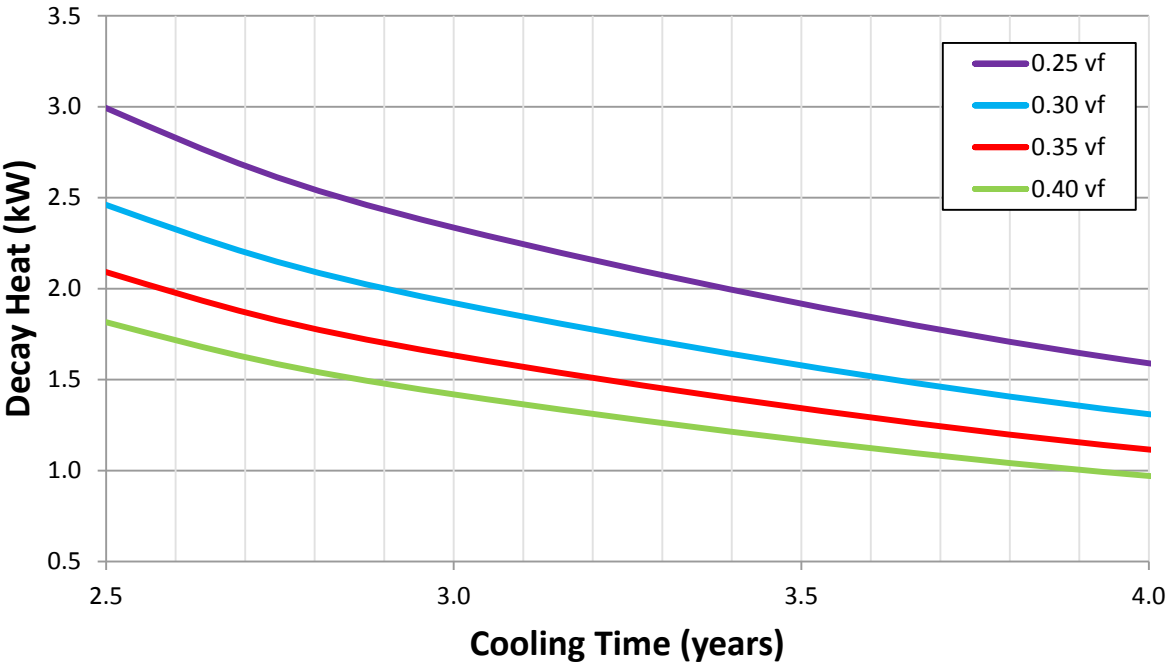

Figure 8. Decay heat generated between 2.5 and 5 years cooling for different packing fractions.

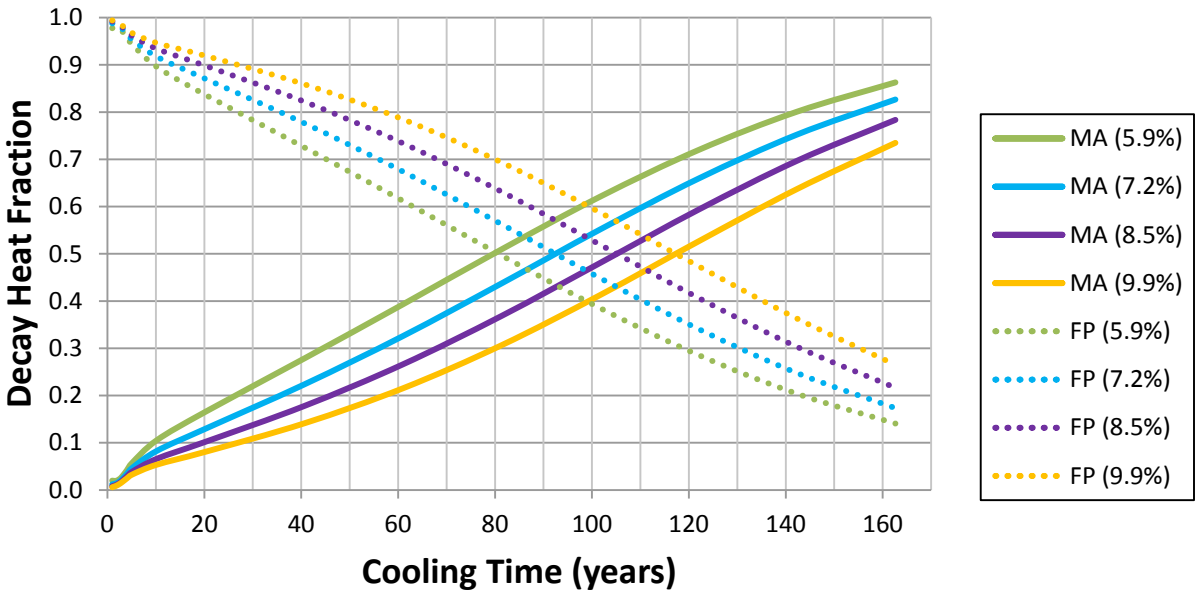

Figure 9. Decay heat fraction from MAs and FPs.

Table 4. Ratio of major FP isotopic contribution to decay heat.

Fission Products	Contribution (%) per Cooling Time					
	10 days	JAEA [5] 10 days	45 days	2 years	5 years	JAEA [5] 5 years
^{85}Kr	0.0	-	0.0	0.3	0.9	0.9
^{89}Sr	4.3	4.0	5.4	0.0	0.0	-
^{90}Sr	0.1	-	0.2	2.0	6.4	5.9
^{90}Y	0.5	-	0.9	9.8	30.5	27.9
^{91}Y	5.8	5.5	7.8	0.0	0.0	-
^{95}Nb	10.9	10.7	19.2	0.2	0.0	-
^{95}Zr	10.4	10.1	14.4	0.1	0.0	-
^{103}Ru	4.8	5.2	5.2	0.0	0.0	-
^{106}Ru	0.0	-	0.0	0.1	0.1	0.1
^{106}Rh	3.9	4.6	7.3	22.0	9.1	11.2
^{125}Sb	0.0	-	0.0	0.3	0.5	0.5
^{131}I	1.8	1.9	0.2	0.0	0.0	-
^{132}I	3.4	3.5	0.0	0.0	0.0	-
^{134}Cs	0.5	-	1.0	6.0	7.1	10.6
^{137}Cs	0.1	-	0.2	2.3	7.2	7.3
^{140}La	25.8	25.5	7.8	0.0	0.0	-
^{140}Ba	4.0	3.9	1.2	0.0	0.0	-
^{141}Ce	2.6	2.6	2.5	0.0	0.0	-
^{143}Pr	2.5	2.5	0.9	0.0	0.0	-
^{144}Pr	11.4	11.0	21.2	43.2	9.4	9.6

Table 4. (continued).

Fission Products	Contribution (%) per Cooling Time					
	10 days	JAEA [5] 10 days	45 days	2 years	5 years	JAEA [5] 5 years
^{144}Ce	1.0	1.0	1.9	3.9	0.8	0.9
^{147}Nd	1.1	1.1	0.2	0.0	0.0	-
^{147}Pm	0.1	-	0.2	1.3	2.0	1.8
^{154}Eu	0.0	-	0.0	0.3	0.8	1.2

Table 5. Ratio of major MA isotopic contribution to decay heat.

Minor Actinides	Contribution (%) per Cooling Time			
	5 years	JAEA [5] 5 years	140 years	JAEA [5] 150 years
^{238}Pu	19.6	18.3	3.7	3.3
^{239}Pu	14.6	19.22	8.1	10.6
^{240}Pu	19.7	15.1	10.8	8.3
^{241}Pu	3.7	3.7	0.0	-
^{241}Am	39.4	39.7	77.2	77.7
^{242}Cm	0.5	0.5	0.0	-
^{244}Cm	2.1	3.2	0.0	-

2.3 RAVEN-Generated Reduced Order Model for Decay Heat Calculation

After the ORIGEN calculations have been performed with the varying input space shown in Figure 12 and Table 6, decay heat curves obtained from these calculations are used to train the specified ROM in RAVEN. Although the main purpose for training a ROM with RAVEN is to be able to predict the decay heat value at any given time as a function of initial/operating conditions, this section shows the feasibility of such a methodology and the main analysis is left as future work. The trained ROM is then tested with a new input space obtained from Monte Carlo sampling of the input space with a uniform distribution. The resulting input space is shown in Figure 13 Note that the two variables in the input space (i.e., specific power and volume fraction) are correlated; therefore a correlation function based on the volume fraction is applied while sampling the specific power.

Table 6. Input space for ORIGEN calculations.

Enrichment (^{235}U wt.%)	Volume Fraction	Specific Power (MW/tHM)
5.9	0.25	40.00
6.5	0.27	37.04
7.2	0.30	33.30
7.8	0.33	30.30
8.5	0.35	28.57
9.2	0.37	27.03
9.9	0.40	25.00

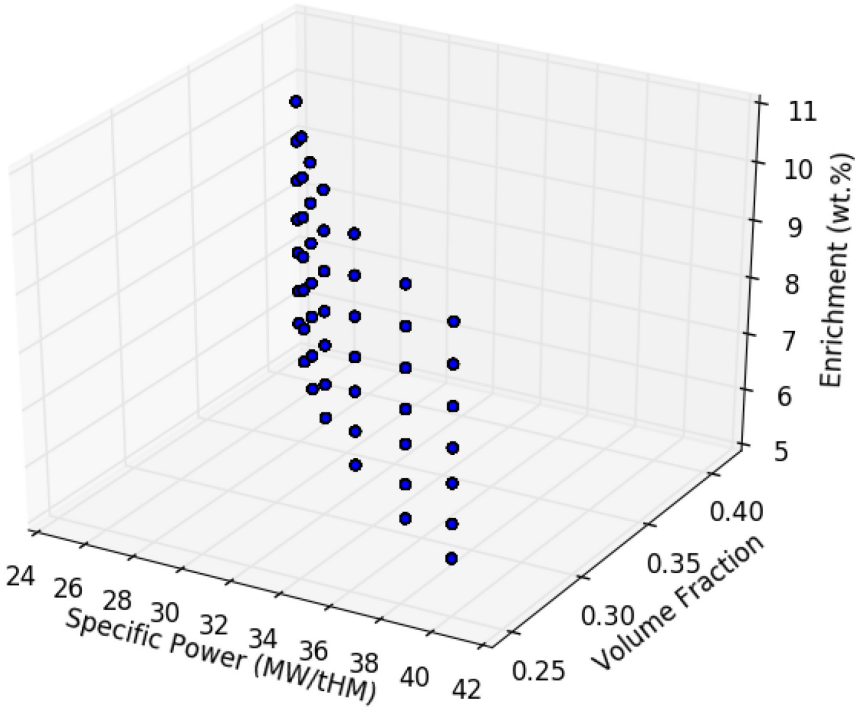

Figure 10. Input space used in the ORIGEN calculations.

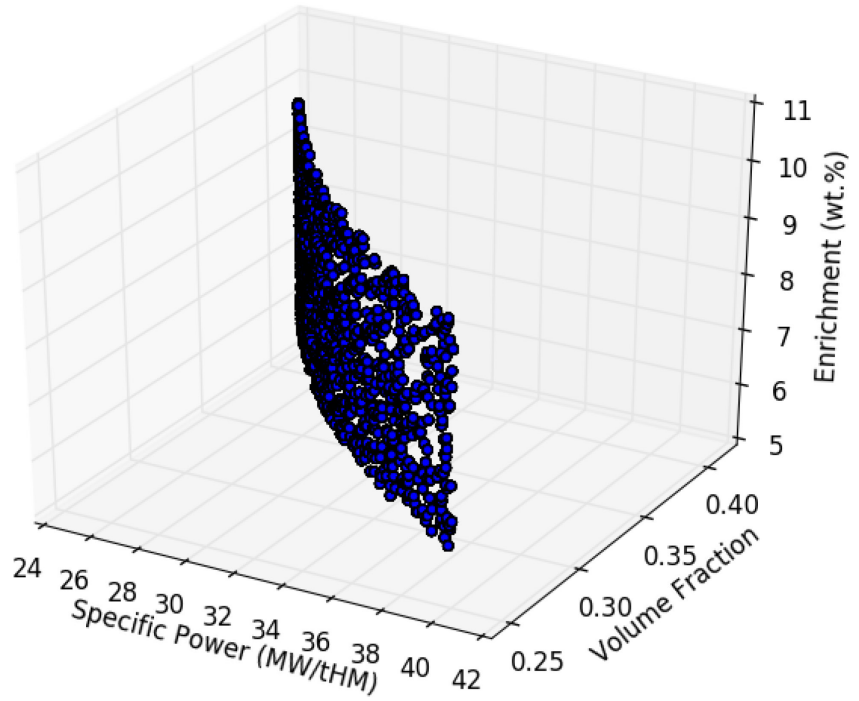

Figure 11. Input space (Monte Carlo Sampling – thousand points) used for ROM testing.

Results from both the ORIGEN calculations and ROM testing are presented in Figure 14 for the entire input space as scattered points and lines, respectively. Results from the ROM test and ORIGEN calculations showed a very good agreement. Figure 13 shows ORIGEN and ROM results for three different enrichments (i.e., 5.9%, 7.5%, and 9.9%) with volume fraction and specific power fixed at 0.3 and 33.3 MW/tHM, respectively. These results show very good agreement and ROM can reproduce the ORIGEN values.

Figure 14 shows ORIGEN and ROM results for two selective cases: (1) with an enrichment of 6.5%, volume fraction of 0.27, and specific power of 37.04 MW/tHM, and (2) with an enrichment of 9.9%, volume fraction of 0.4, and specific power of 40 MW/tHM. Figure 14 also shows separate ROM results for a case that is not in the training set (i.e., with an enrichment of 7.5%, volume fraction of 0.36, and specific power of 27.78 MW/tHM). The ORIGEN and ROM results show very good agreement and ROM is able to reproduce the ORIGEN results and another case that is not available in the training set.

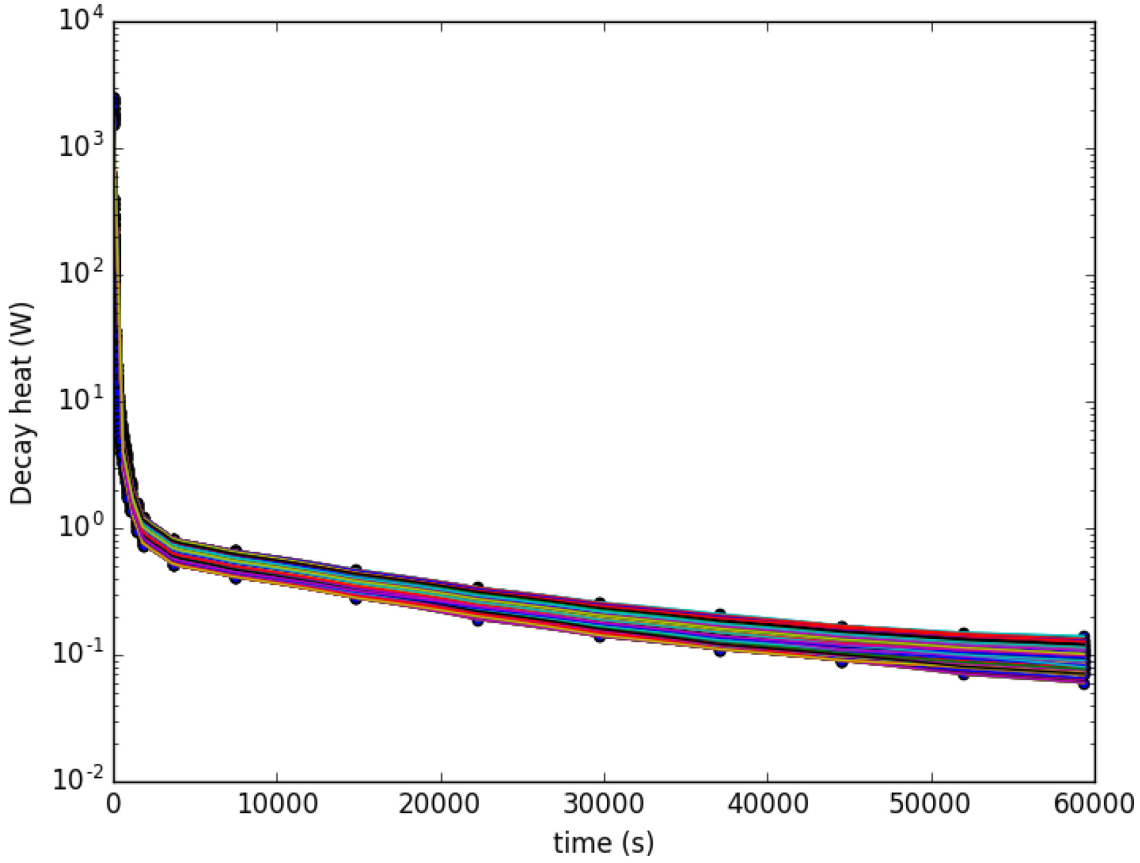

Figure 12. Results of ORIGEN (scattered) and ROM (lines) simulations.

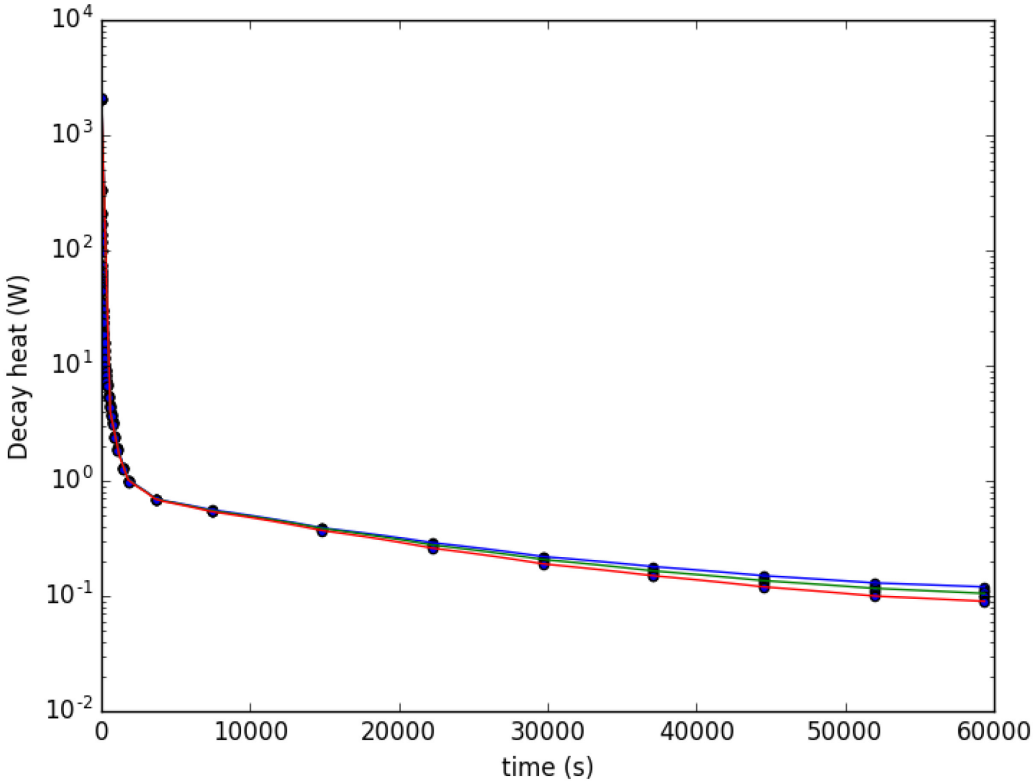

Figure 13. ORIGEN (scattered) and ROM (lines) results for different enrichments.

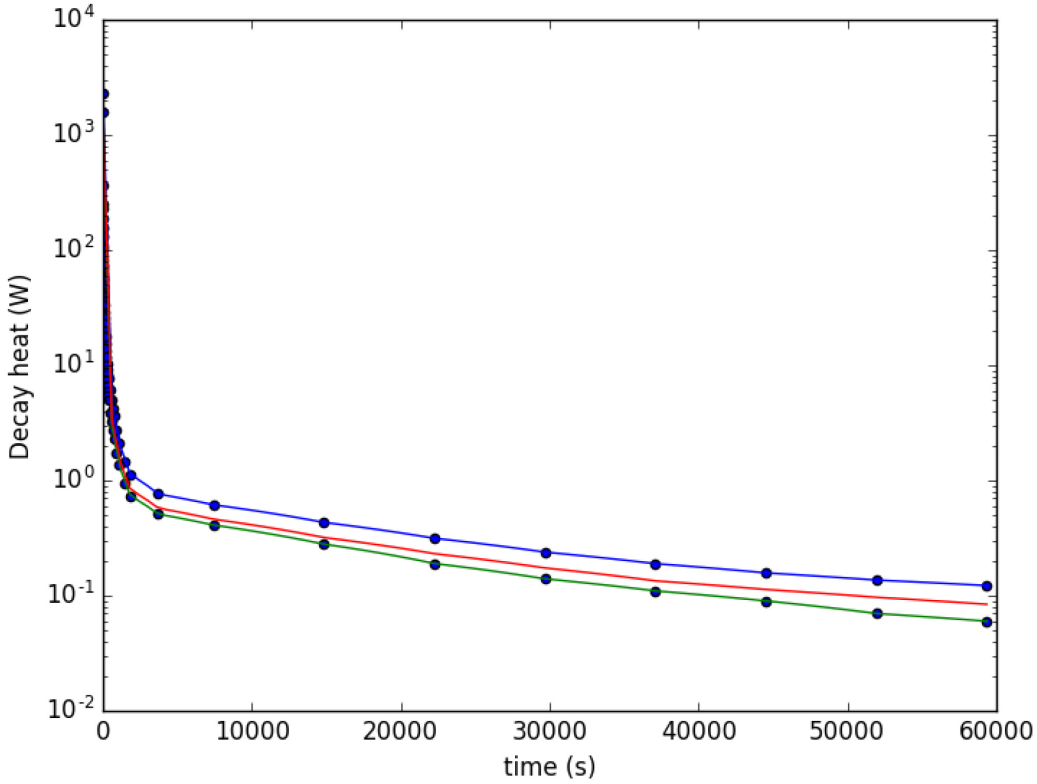

Figure 14. Results of ORIGEN and ROM for selective cases.

3. CONCLUSION

A two-dimensional HTTR fuel assembly block was modeled using the SCALE 6.2 package. The ORIGEN module was used to generate HTTR-specific cross-section libraries to be used for subsequent decay heat analysis over a range of fuel enrichments, fuel temperatures, and TRISO particle packing fractions with the appropriate specific power. The results demonstrate very good agreement with a previous study done by JAEA using the same fuel enrichment, fuel temperature, and packing fraction. A database of generated HTTR libraries can be used in the future to quickly analyze decay heat following normal or transient operation. Comparison of ORIGEN and ROM results showed that the trained ROM in RAVEN can be used for calculating the decay heat for those cases that are covered by the input space. Because the input space in the training set was limited and had two dependent variables, coverage of the trained ROM is limited. In future work, the training input space dimensions will be increased to include temperature and burnup, thus eliminating the direct dependence of specific power on volume fraction. Additionally, the fractional contribution to decay heat, whether from MAs or FPs, could be added to the input space to better quantify the decay heat precursors. Finally, time is currently in the output space (i.e., decay heat values can only be generated on certain time values while using ROM). However, it is possible for the RAVEN code to be used to transform the time from output space to input space, which is also left as future work.

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