INL/EXT-21-64242

Initial study on cross section generation requirements for a PBR equilibrium core

September 2021

ART - M3AT-21IN0601011

Javier Ortensi[1] and Paolo Balestra[1]

[1]*Idaho National Laboratory*

INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance, LLC

INL/EXT-21-64242

Initial study on cross section generation requirements for a PBR equilibrium core

ART - M3AT-21IN0601011

Javier Ortensi[1] **and Paolo Balestra**[1]

[1]**Idaho National Laboratory**

September 2021

Idaho National Laboratory
Advanced Reactor Technologies
Idaho Falls, Idaho 83415

http://www.art.inl.gov

Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

Page intentionally left blank

ART Program

Initial study on cross section generation requirements for a PBR equilibrium core

INL/EXT-21-64242

September 2021

Technical Reviewer: (Confirmation of mathematical accuracy, and correctness of data and appropriateness of assumptions.)

Ryan Stewart — 9/1/2021

Ryan H. Stewart — Date
Nuclear Engineer

Approved by:

M. Davenport — 09/01/2021

Michael E. Davenport — Date
ART Project Manager

Gerhard Strydom — 8/31/2021

Gerhard Strydom — Date
ART National Technical Director

Michelle Sharp — 8/31/2021

Michelle T. Sharp — Date
INL Quality Assurance

Page intentionally left blank

PHYSOR 2022: Making Virtual a Reality - Advancements in Reactor Physics
To Leap Forward Reactor Operation and Deployment
Pittsburgh, Pennsylvania, USA, May 15th-20th, 2022

Initial study on cross-section generation requirements for a PBR equilibrium core

Javier Ortensi[1]*,**Paolo Balestra**[1]

[1]Idaho National Laboratory

javier.ortensi@inl.gov

ABSTRACT

A Serpent model of the equilibrium core HTR-PM, a small modular nuclear reactor under development in China, was developed for use in cross-section preparation studies in order to guide methods development for the Griffin reactor multiphysics application. The model includes detailed isotopics for 10 distinct pebble burnup groups in 126 core zones with unique fuel and moderator temperatures obtained from a coupled neutronics-thermal-fluids equilibrium core calculation using Griffin-Pronghorn. A sensitivity study of the fuel and moderator temperatures for various core regions was performed with the MOOSE stochastic tools. The results show that the uncertainties are, not unexpectedly, dominated by the value of the fluid temperature and that the power level, heat transfer coefficient and effective conduction to neighboring pebbles and fluid constitute, at best, second order effects. The temperature uncertainty range varies from 28 K to 57 K at the core entry and exit planes, respectively, but these values are probably higher. We still have to quantify the significance of these uncertainties in the preparation of cross-sections in future work. In addition, we verified that the effective pebble approximation used in the PEBBED and V.S.O.P. computer codes works well for the preparation of region averaged cross-sections. Nevertheless, there are some discrepancies in the cross-sections when compared to the multi-pebble model, which could affect the prediction of peak values and the depletion calculation. We conclude that is highly desirable for future studies with Griffin to be able to handle both the "effective" pebble approximation and the multi-pebble approach for various pebble burnup groups. This enables Griffin users with the flexibility to perform higher-fidelity studies. Finally, we initiated the preparation of cross-sections for various core regions from the full core Serpent reference model. We quantified the differences in 26 group cross-sections from infinite domain models. These reference cross-sections will serve to validate the double heterogeneity, self-shielding, and spectrum-correction methods in Griffin.

KEYWORDS: Serpent, Griffin, PBR, HTR-PM

1. INTRODUCTION

The process of preparing broad group neutron microscopic cross-sections in any system relies on the accuracy of the energy spectrum, since it is used as the weighting function in the group condensation step. There are two general approaches for the preparation of nuclear data: (1) deterministic methods that rely on a number of approximations to determine the neutron spectrum; and (2) modern Monte Carlo methods, which provide an avenue to model the exact geometry without energy, angular, and spatial discretization

*corresponding author

errors. Griffin [1] is a reactor multiphysics application developed jointly by both Idaho National Laboratory and Argonne National Laboratory. Griffin includes the cross-section Application Programming Interface (CSAPI) [2], which falls in the first category. Yet there are other Pebble-Bed Reactor (PBR) specific methods that might be required to prepare cross-sections. Fortunately, there is a significant amount of literature on potential approaches to the preparation of broad-group homogenized cross-sections for PBRs. The treatment of the heterogenity in the TRi-structural ISOtropic (TRISO) particle and pebble has been adopted in a number of deterministic computer codes [3–6], including Griffin [2]. In addition, various Monte Carlo codes can model the explicit geometry [7–10] and prepare cross-sections, but computing a reference equilibrium core requires further progress. There is consensus between the various experts that challenges still remain in: (1) the coupling of the various core regions due to the long neutron migration lengths; and (2) the random nature of the pebble distribution in the core.

The challenge with (1) is traditionally treated in deterministic full core simulators with a leakage correction to coarse broad-group energy cross-sections with the aim to reduce the computational burden [11,12]. A review of the various leakage correction methods is provided in [13]. In his work, D. She shows that the new improved iterative feedback method performs well to obtain a better eigenvalue, but is not sufficiently substantiated with appropriate figures of merit (i.e., rms and maximum values in the flux, reaction rates, or power distributions). In a separate study, Gougar [14] confirms that the effectiveness of the leakage correction is very sensitive to the group structure and generally provides a clear advantage for coarse broad-group structures (< 6 energy groups). In this same study, Gougar used a 26 group structure that appears to consistently outperform any form of leakage correction for coarser broad-group structures in single and multi-composition cores. Missing from these comparisons are the study of potential sources of cancellation of error in the integral quantities, normally used as figures of merit, and the effects from fuel and moderator temperatures across the core, which impact the neutron leakage across the core and the effectiveness of the neutron leakage correction.

With regard to (2), one of the major points of contention emerge in the treatment of pebbles of different types or burnup histories within a spectral zone. The approach used in the computer codes V.S.O.P. [11] and PEBBED [12] assumes that a single ”effective” pebble within the spectral zone is sufficient to treat the local spatial and energy self-shielding effects of all pebbles in that zone through the use of a multi-layer model. The multi-pebble self-shielding implementation in the APOLLO2 code [15] sought to improve upon the ”effective” pebble model by treating the pebble-to-pebble and pebble-to-coolant interactions. The APOLLO2 approach was tested with a highly heterogeneous experiment conducted at the ASTRA critical facility in the National Research Center Kurchatov Institute. The APOLLO2 approach showed good agreement in the eigenvalue compared to the ”effective” pebble, but had mixed results with reaction rate comparisons. This work was later extended [16] and showed that for a low-enriched uranium (LEU) core composition the main difference between the two approaches was in the plutonium resonances. A different multi-pebble implementation in the PANGU code [17] has shown that there are significant issues in the ”effective” pebble model with higher pebble heterogeneity.

These studies have been primarily focused on how to obtain the optimal flux weighting spectrum in predefined fixed spectral zones. What appears to be missing from these papers is a fundamental question on how well we know the uncertainty in the parameters on which the cross-sections depend. For most high-temperature reactor applications the cross-sections are tabulated as a function of fuel and moderator temperature. It is highly desirable to match the resolution of the neutronics solution to that of the thermal fluids as to optimize the computational effort. Current work with Serpent [18] has examined the variation of one group cross-sections as they apply to core depletion due to power level, burnup, and fuel and moderator temperatures. But that is insufficient for modern deterministic codes that compute the reactor rates for their Bateman solvers from the broad group scalar fluxes and cross-sections.

The primary purpose of this work is to develop a high-fidelity Serpent equilibrium core model of the HTR-PM to study the cross-section preparation methods needed for gas-cooled PBRs. These methods will later be implemented in the Griffin workflow. In addition, other goals of the research include: (a) the determination of the fuel and moderator sensitivity in pebble and TRISO thermal fluids calculations, which

can latter be used to ascertain the level of accuracy required in the neutronics self-shielding calculations; (b) the verification of the effective pebble approximation for a typical gas-cooled PBR; and (c) the comparison of cross-sections prepared with an infinite domain approximation to the full core values with continuous energy Monte Carlo.

2. ANALYSIS METHODOLOGY

To build a high-resolution Serpent model, we require the isotopic compositions for each pebble type in each core zone and their corresponding fuel and moderator temperatures. This data can be obtained from a coupled multiphysics equilibrium core calculation using Griffin-Pronghorn, which is discussed in Section 2.1. The sensitivity analysis for the fuel and moderator temperatures in presented in Section 2.2. Finally, in Section 2.3, we introduce some details in the development of the Serpent reference equilibrium core model.

2.1. GRIFFIN-PRONGHORN EQUILIBRIUM CORE MODEL

The Griffin-Pronghorn model from [19] was improved to the specifications shown in Table I. It is a core-zone homogenized R-Z model. The mesh is shown in Figure 1, where we identify the various material zones as well as six regions of interest (ROI) for later analysis. The Griffin model employs 9 group microscopic cross-sections for 294 isotopes obtained from the DRAGON [20] code assuming an infinite domain calculation. As we will later show, this approach is fundamentally flawed, but it serves to produce the initial cross-section set that will be later improved with the new Griffin capabilities. The DRAGON model was improved from that used in [19] to represent a pebble ensemble with a fresh pebble surrounded by burned pebbles at a core burnup of 53.08 GWd/MT. In this initial study, the cross-sections are parameterized as shown in Table I. The top void transport cross-sections were calculated in Serpent with the cumulative migration method [21].

Table I: HTR-PM Model Specifications.

Parameter	Value
Core Power [MWth]	250
Number of Pebbles	419,384
Pebble packing fraction (average)	0.61
Number of particles per pebble	11,660
Pebble bed radius [m]	1.5
Pebble bed height [m]	11.0
Pebble types	1 pebble type (7g IHM)
Number of passes	15
Number of streamlines	6 (equally spaced)
Number of burnup groups	10 (from 0-100 at 10 GWd/MT intervals)
Pebble Residence time [days]	70.5
Discharge burnup [GWd/MT]	90
Burnup tabulation [GWd/MT]	0, 22.0, 53.08, 73.77, 99.05
Fuel temperature tabulation [K]	500.0, 700.0, 900.0, 1100.0, 1300.0
Moderator temperature tabulation [K]	300.0, 500.0, 700.0, 900.0, 1100.0, 1300.0

Pronghorn uses the continuous finite element method (FEM) porous medium solver to determine the thermal-fluid fields. The 1-D pebble and TRISO conduction models from [19] were modified by changing the pebble boundary condition (BC) from a Dirichlet to one Neumann and one Robin. The initial Dirichlet

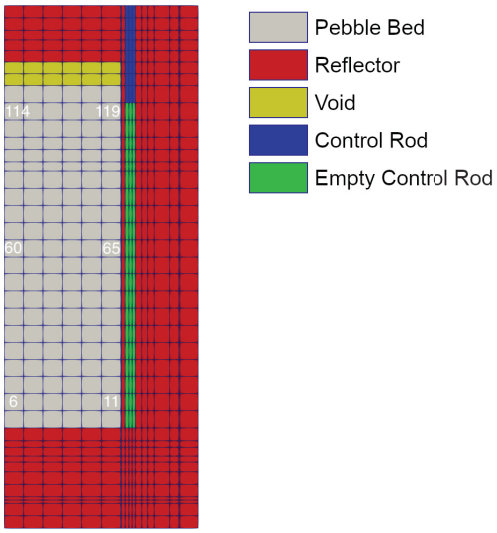


Figure 1: Simplified Griffin model of the HTR-PM. The numbers indicate the pebble bed element of interest for cross-sections.

BC had a value set to the average surface temperature of all pebbles in that core zone. The new Neumann BC is set to the average heat flux in the solid material for each core zone,

$$q"_{solid} = -k_s \nabla T_{solid}, \tag{1}$$

where T_{solid} is the Pronghorn solid temperature solution and k_s is the "stagnant" effective thermal conductivity. This conductivity takes into account the heat transferred between the pebbles and a stagnant fluid in that zone [22]. Currently, the value of k_s is overestimated since it also includes intra-pebble conductivity. This means that additional heat is removed from the pebble and TRISO energy conservation equations and that the temperature values would tend to be higher.

The Robin condition,

$$q"_{solid} = h(T - T_{fluid}), \tag{2}$$

couples the pebble surface temperature (T) to the average bulk fluid temperature T_{fluid} in that zone through the heat transfer coefficient (htc) h.

The thermophysical properties for the various TRISO layers and the pebble graphite matrix were updated to include temperature, burnup, and fluence dependence per the values in [23]. In the simulation, Griffin transfers the pebble burnup based on the pebble burnup group. Therefore, groups 0-9 correspond to average burnups between 5 and 95 in 10 GWd/MT steps. The burnup value in fissions per initial metal atom (FIMA) and fast DIDO [24] equivalent fluence are computed with the following equations derived from the DRAGON depletion calculations:

$$FIMA = -2.022642 \times 10^{-6} * B^2 + 1.053601 \times 10^{-3} * B \tag{3}$$

$$fluence = 7.41611 \times 10^{-6} B^3 - 5.36979 \times 10^{-6} B^2 + 1.37527 \times 10^{-2} B - 4.48921 \times 10^{-2} \tag{4}$$

where B is the burnup in GWd/MT and the fluence is in $n/m^2 \times 10^{25}$.

2.2. SENSITIVITY OF THE FUEL AND MODERATOR TEMPERATURES

The reactivity feedback mechanisms in graphite-moderated reactors with LEU or high-assay low-enriched uranium (HALEU) fuel are dominated by temperature changes in fuel and graphitic materials. Doppler broadening of the fuel cross-sections leads to a strong and instantaneous feedback that closely follows any power changes. Neutron spectral shifting and transition of the thermal peak into a higher energy effectively reduces the fission events in the 1/v region, thus generally leading to higher leakage from pebble-bed zones. It also leads to negative feedback lower in magnitude than Doppler broadening and with a longer time constant due to the high heat capacity of graphite. The graphite reactivity feedback can be positive, but small, in reflector regions, in events where the reflectors heat up. Given the importance of these two parameters we would like to better understand the uncertainty on both for the equilibrium core HTR-PM model. This can help us to better understand the accuracy necessary for the preparation of neutron cross-sections.

For this task, we deployed the MOOSE-based stochastic tools [25]. We perform a sensitivity analysis on various parameters that are used as inputs in the pebbled and TRISO models described in Section 2.1. The parameters that we focused on are listed in Table II with their uncertainties. The uncertainties on the parameters were selected based on the current PBRs modeling experience [26–28]. Note that each parameter is treated as an independent variable in the stochastic tools. Several inputs are prepared, one for each of the parameters treated separately and one case with all parameters combined. Each input is executed for each of the zones of interest identified in Section 2.1. A python script loads the Griffin-Pronghorn output files from the equilibrium core calculation and execute the various inputs by providing the local mean and standard deviation (based on the uncertainties in Table II). All calculations use a Latin hypercube sampling (LHS) with 1000 samples. A significant limitation of this calculation is that we do not for the interdependence of the various parameters. The power density depends on the fuel and moderator temperatures through their effect on the cross-sections, and thus the flux. Similarly, the rest of the parameters depend on the local power through the solid temperature. In the future, we plan to perform sensitivity calculations on the full core Griffin-Pronghorn model to account those effects.

Table II: Parameters and used in the fuel and moderator temperature sensitivity study for the pebble bed.

Parameter	Uncertainty
Power density	2.5%
Heat transfer coefficient (htc)	5 and 20%
Fluid temperature	5%
Effective heat flux	5%

2.3. SERPENT EQUILIBRIUM CORE MODEL

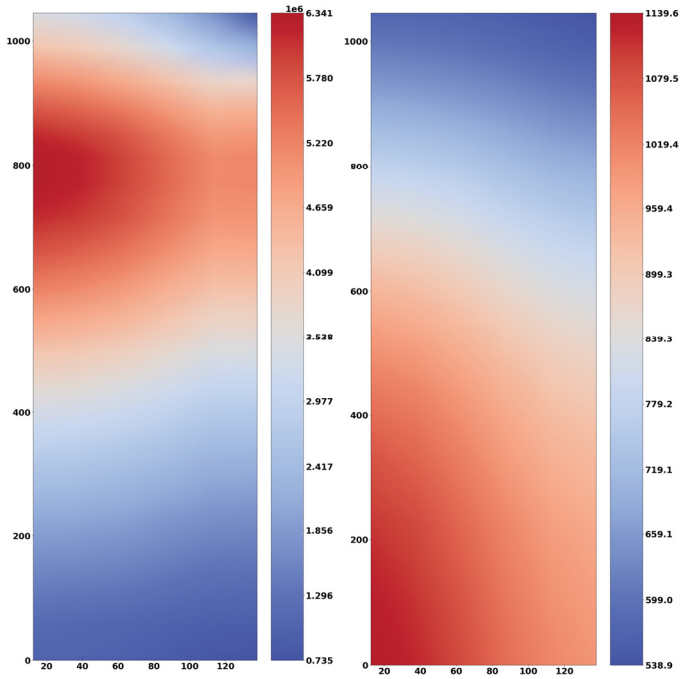
The Serpent model uses the explicit, random pebble and TRISO distributions. We developed a stochastic distribution of pebble types, based on their burnup, for each core zone, which approximate the packing fraction obtained from the Griffin solution. The core zone assignment is based on the centroid of the pebble. The 294 isotopes from the Griffin solution are assigned to each TRISO particle in each pebble burnup type for each core zone leading to an approximate equilibrium core model with which to study neutron cross-sections. Note that the packing fractions in Serpent and Griffin are not exactly the same for two reasons. 1). Griffin currently assumes a constant packing fraction of 0.61, whereas Serpent uses an explicit pebble distribution with variable packing. For the regions of interested (6-119), in ascending order, the packing fractions are 0.6168, 0.6069, 0.6095, 0.6156, 0.6022, and 0.6047, respectively. 2). Serpent

pebbles are discrete entities whereas the Griffin packing fractions are based on averaged values for each pebble burnup group.

The Serpent model contains 1260 distinct pebble/TRISO compositions with unique fuel and moderator temperatures. The other materials in the model were also assigned consistent solid temperatures with those of Pronghorn solution. We generate models that represent an infinite domain by bounding the Serpent full core model with surfaces consistent with the Griffin mesh and assigning a reflective boundary condition. The models close to the reflector (e.g., regions 11, 65, and 119) extend into the reflector in an attempt to include reflector effects in the infinite medium calculation. These models allows us to compare the full core calculation to a more local infinite domain calculation that is representative of a traditional lattice physics code. For the infinite domain models, we have two variants—one with 10 pebble burnup types and one with a single "effective" or representative pebble with the average isotopics and temperatures. We compute spectra in 167 groups [3] and cross-sections in 26 group [14] for each zone.

3. RESULTS

The power and solid temperature solutions from the coupled Griffin-Pronghorn equilibrium core model are shown in Figure 2. The power distribution is consistent with published results using the Very Superior Old Programs (V.S.O.P) [29]. The power exhibits a characteristic shape with the power peak shifted towards the top of the core due to both the lower temperatures and burnup. The solid temperature exhibits a ~ 600 degree gradient in the axial direction.



(a) Power Density $[W/m^3]$ **(b) Solid Temperature** $[K]$

Figure 2: Griffin solutions for the equilibrium core HTR-PM (pebble bed).

Results from the sensitivity of the fuel temperature to the various parameters are shown in Table III. The largest contributor to the uncertainty in the fuel and moderator temperatures, not unexpectedly, is the fluid temperature. The change in the gradient between the surface temperature and the bulk fluid directly relates to a similar change in the fuel and moderator temperatures. The power level, htc, and the heat transfer

to other pebbles play a less important role in the steady state. This changes during loss-of-forced-cooling transient scenarios where the the latter plays a dominant role. We will leave that challenge to future studies. The results from the sensitivity to all parameters are included in Table IV for the fuel and moderator temperature. The values are averaged among the various pebble types in the zone, since the temperatures and standard deviations were not significantly different. The results show that the uncertainty in the temperature ranges from 28 K to 57 K for the entry and exit core planes, respectively.

Table III: Sensitivity of the fuel temperature [K] ($\pm 1\sigma$) for each independent parameter in pebble burnup group 5. Similar sensitivies are observed for the moderator temperature and other pebble burnup groups.

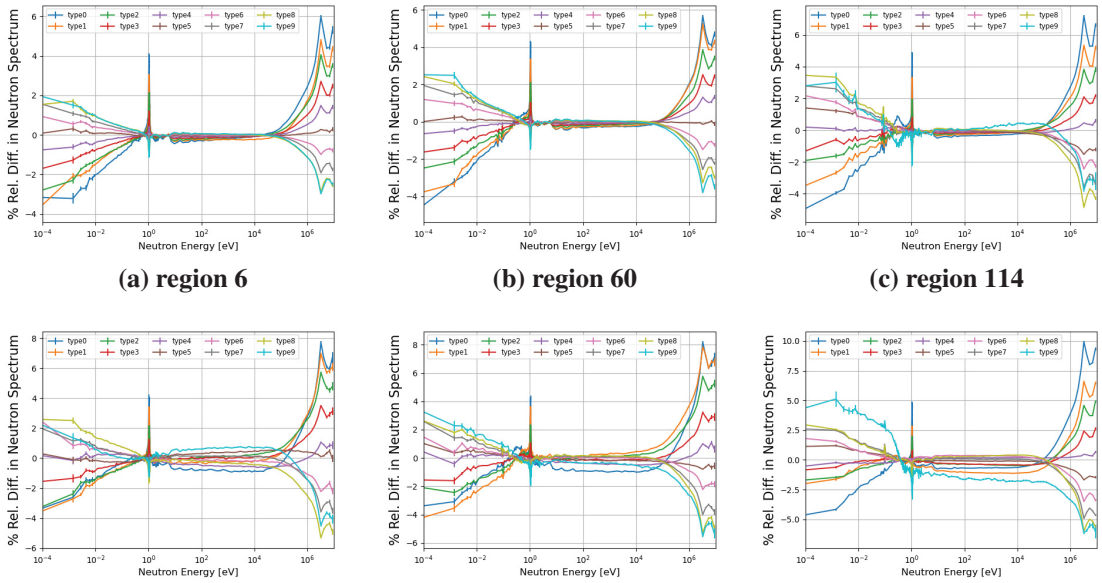
parameter	R6	R11	R60	R65	R114	R119
power (2.5%)	1153.4 (0.7)	1003.1 (0.5)	1048.0 (2.7)	904.2 (2.0)	659.4 (2.0)	584.4 (1.0)
tfluid (5%)	1153.4 (56.9)	1003.1 (49.6)	1048.0 (49.3)	904.2 (42.8)	659.4 (30.2)	584.4 (27.8)
htc (5%)	1153.5 (0.4)	1003.1 (0.3)	1048.1 (1.8)	904.2 (1.4)	659.5 (1.7)	584.5 (0.9)
htc (20%)	1153.8 (1.97)	1003.4 (1.51)	1049.6 (8.46)	905.4 (6.60)	661.0 (8.15)	585.2 (4.13)
hflux (5%)	1153.4 (0.01)	1003.1 (0.01)	1048.0 (0.02)	904.2 (0.01)	659.4 (0.01)	584.4 (0.01)

Table IV: Sensitivity of the fuel and moderator temperature [K] ($\pm 1\sigma$) averaged over all burnup groups for each ROI. Based on perturbation of all independent parameters. Similar sensitivies are observed for the other pebble burnup groups.

	R6	R11	R60	R65	R114	R119
fuel	1153.35 (56.9)	1003.0 (49.6)	1047.8 (49.5)	903.8 (42.9)	659.7 (30.4)	584.4 (27.9)
moderator	1144.15 (56.6)	996.3 (49.4)	1012.4 (48.4)	877.6 (42.1)	636.3 (29.8)	573.1 (27.6)

Plots of neutron spectra are provided in Figure 3 to better understand the difference between an infinite homogeneous medium calculation with a variety of pebbles at different burnups and that of the effective pebble approach. The largest differences are observed near the top of the core (regions 114 and 119), where the fuel and moderator temperatures are less homogeneous. There are significant discrepancies in the high and low energy regions with a distinct peak near 1 eV, which was also observed in Grimod's work [16], but not well qualified. There are several resonances near 1 eV, including ^{235}U and ^{240}Pu fission and capture. This is clearly shown in Figure 4. Note that the average ^{235}U number densities in the ROI are 10-15 times larger than ^{240}Pu. Nevertheless, the ^{240}Pu capture reaction rates will be larger in high burnup pebbles due to the magnitude of the cross-section. We also observe a larger difference in various energy ranges for regions near the reflector, particularly for high burnup pebbles in region 119.

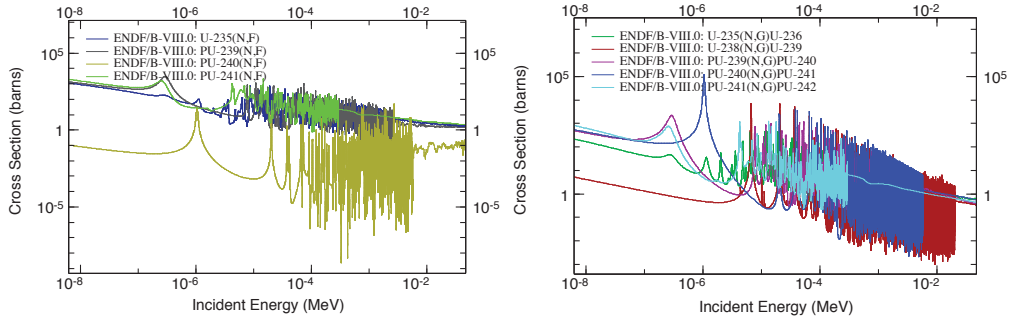
To compare the accuracy of the cross-section averaging process, we computed 26 group cross-sections for various isotopes and burnup group in the infinite domain. The plots in Figure 5 and 6 include the % relative differences between the cross-sections of each burnup type and the effective pebble cross-section. The second plot that we include is the % relative differences in the average cross-section that is computed with the number densities and pebble volumes in that core zone. The results from the effective pebble approximation show good agreement with these averaged values. We include one harder spectrum zone in Figure 5, and a softer spectrum in Figure 6, because they show the largest discrepancies in the data. The averaging process tends to smear the differences in the individual pebble cross-sections, which can potentially lead to miss-predictions in the pebble peak power and temperature. We observe significant differences in the



(a) region 6 **(b) region 60** **(c) region 114**

(d) region 11 **(e) region 65** **(f) region 119**

Figure 3: Comparison of neutron spectra in each burnup group compared to the effective pebble approach for an infinite medium calculation. Error bar = $\pm 1\sigma$.

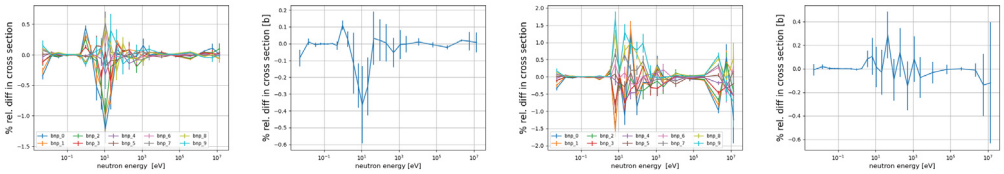


(a) neutron fission **(b) neutron capture**

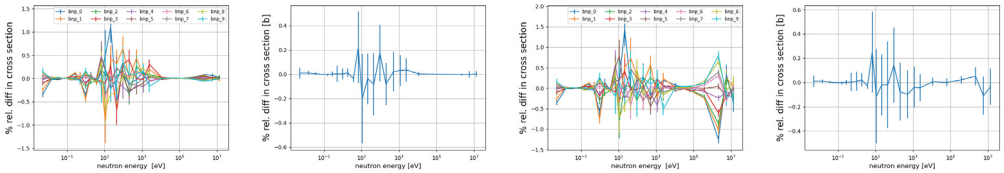
Figure 4: Cross-sections for various isotopes near the 1 eV range. [30]

highest burnup group at the core entry plane near the reflector (region 119). Even though the averaged cross-sections agree well, we can conclude that it is highly desirable to include both approaches in the Griffin workflow to provide the ability to perform low and high fidelity studies.

Finally, we compare 26 group cross-sections computed with an infinite domain versus those prepared via a full core calculation. Four key isotope reactions are shown in Figures 7 and 8. We first focus on the region where we expect the infinite domain calculation to perform well—region 60. This zone has a harder neutron spectrum due to the position with respect to the reflectors. The results indicate that ^{235}U fission is over and under estimated in different energy ranges, which could produce cancellation of error and potentially the improved integral solutions observed in [14]. ^{238}U capture is significantly and consistently underestimated in all pebble burnup types. This is expected since the ^{238}U number densities remain nearly constant in LEU

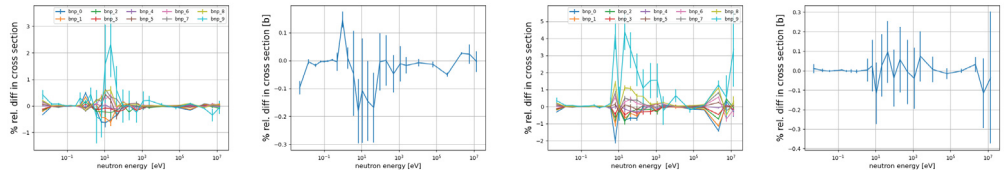


(a) U235 fission **(b) U235 fission - averaged** **(c) U238 capture** **(d) U238 capture - averaged**

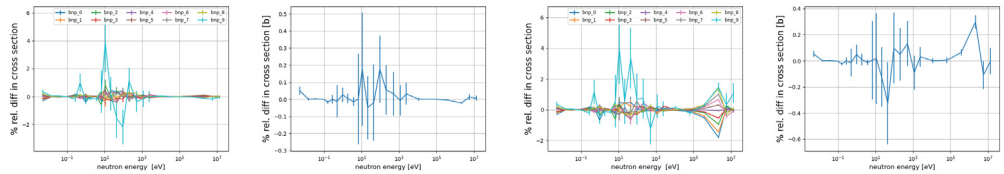


(e) Pu239 fission **(f) Pu239 fission - averaged** **(g) Pu239 capture** **(h) Pu239 capture - averaged**

Figure 5: Accuracy of the effective pebble approximation for various isotopes in 26 energy groups (region 60). Error bar $\pm 1\sigma$.



(a) U235 fission **(b) U235 fission - averaged** **(c) U238 capture** **(d) U238 capture - averaged**

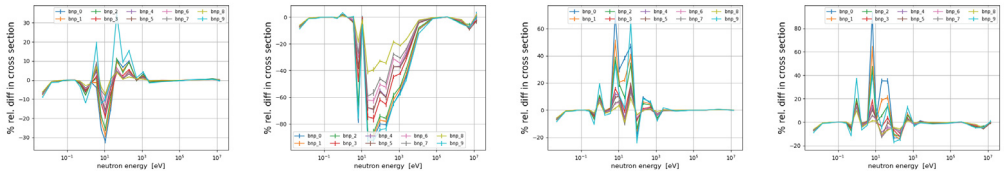


(e) Pu239 fission **(f) Pu239 fission - averaged** **(g) Pu239 capture** **(h) Pu239 capture - averaged**

Figure 6: Accuracy of the effective pebble approximation for various isotopes in 26 energy groups (region 119). Error bar $\pm 1\sigma$.

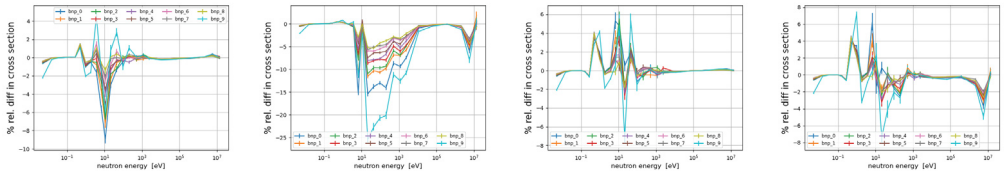
fuel. With regard to ^{239}Pu fission and capture, there is significant overprediction of the cross-section in the various resonances, specially at 0.295 eV.

The cross-sections in the thermal spectrum zone (region 65) have errors lower in magnitude. Recall that the infinite domain calculation includes 30 cm of reflector, which produces a better approximation of the spectrum. The pebbles in the higher burnup group dominate both the error and uncertainty of the calculation. Here again, we observe variability in ^{235}U fission, and the underprediction of the ^{238}U capture, whereas the ^{239}Pu fission and capture show variability with both over and under predictions.



(a) ^{235}U **fission** **(b)** ^{238}U **capture** **(c)** ^{239}Pu **fission** **(d)** ^{239}Pu **capture**

Figure 7: Comparison of cross-sections prepared with an infinite domain versus a full core model in the core center (region 60). Error bar $\pm 1\sigma$.



(a) ^{235}U **fission** **(b)** ^{238}U **capture** **(c)** ^{239}Pu **fission** **(d)** ^{239}Pu **capture**

Figure 8: Comparison of cross-sections prepared with an infinite domain versus a full core model near side reflector region (region 65). Error bar $\pm 1\sigma$.

4. CONCLUSIONS

A Serpent model of the HTR-PM equilibrium core was developed for use in cross-section preparation studies. The model includes explicit pebble and TRISO particles with detailed isotopic compositions for 10 distinct pebble burnup groups. Each pebble type includes a unique fuel and moderator temperature. The isotopic composition, as well as the temperatures, were obtained from a Griffin-Pronghorn equilibrium core calculation. The fidelity of this model is a bit questionable, since the initial cross-section set was obtained from infinite domain calculations, which we have shown to be a poor approximation for core depletion calculations. Nevertheless, this model servers as an initial point from which to build the PBR cross-section capabilities in Griffin.

A sensitivity study of the fuel and moderator temperatures in various zones of the HTR-PM shows that the uncertainties are clearly dominated by the value of the fluid temperature and that the power level, heat transfer coefficient and effective conduction to the neighboring pebbles, and ”stagnant” fluid are second order effects. The range of uncertainty is from 28K to 57K at the core entry and exit planes respectively, but this value is expected to be higher since the heat transfer by conduction is overpredicted in the current model.

We have also shown that the ”effective” pebble approximation in codes like PEBBED and V.S.O.P. produces good averaged cross-sections, even in the case where the pebble temperatures and burnups are different. But , this approach falls short when the user is interested in peak values, like power or fluence. We can conclude that is highly desirable for future studies with Griffin to be able to handle both the ”effective” pebble approximation and the multi-pebble approach for the various pebble burnup groups. This will allow Griffin users to have the flexibility to perform higher-fidelity studies.

Finally, we have quantified the error in the cross-sections prepared with an infinite domain approximation against a full core calculation with Monte Carlo. It is clear and well-documented in the literature that there

are significant long range effects on the neutron spectrum from other core zones. One of the remaining questions from this work is the impact of the uncertainty in the fuel and moderator temperatures versus the spectrum correction. This will be studied in future work.

ACKNOWLEDGEMENTS

This research made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

This work is supported by the Department of Energy (DOE) Advanced Reactor Technologies Program at Idaho National Laboratory under the U.S. Department of Energy Contract DE-AC07-05ID14517.

REFERENCES

[1] C. Lee and Y.S. Jung and H. Park and E.R. Shemon and J. Ortensi and Y. Wang and V.M. Labouré and Z. Prince, "Griffin Software Development Plan," Research Report INL/EXT-21-63185, ANL/NSE-21/23, Idaho National Laboratory, Argonne National Laboratory, 6 2021.

[2] H. Park and W.S. Yang and C. Lee and Y.S. Jung, "Preliminary Study on TRISO Fuel Cross Section Generation," Research Report ANL/NSE-20/54, Argonne National Laboratory, 9 2020.

[3] W.Y. Yoon and R.A. Grimesey and D.W. Nigg and R.L. Curtis and H.D. Gougar, "COMBINE7.1 -A Portable ENDF/B Version 7-Based Neutron Spectrum and Cross-Section Generation Program," Technical Report INL/EXT-08-14729, Rev. 2, Idaho National Laboratory, 8 2011.

[4] R. Sanchez and G.C. Pomraning, "A Statistical Analysis of the Double Heterogeneity Problem," *Ann. Nucl. Energy*, vol. 18, p. 371, 1991.

[5] A. Hébert , "Scattering Reduction of the Double-Heterogeneity Treatment in Dragon," *Nuclear Science and Engineering*, vol. 160(2), pp. 261–266, 2008.

[6] M.L. Williams and S. Choi and D. Lee , "A New Equivalence Theory Method for Treating Doubly Heterogeneous Fuel–I: Theory," *Nuclear Science and Engineering*, vol. 180(1), pp. 30–40, 2015.

[7] J. Leppänen,, *Development of a New Monte Carlo Reactor Physics Code*. PhD thesis, Helsinki University of Technology, 2007.

[8] Paul K. Romano and Nicholas E. Horelik and Bryan R. Herman and Adam G. Nelson and Benoit Forget and Kord Smith, "OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development," *Ann. Nucl. Energy*, vol. 82, p. 90–97, 2015.

[9] K. Wang, Z. Li, D. She, J. Liang, Q. Xu, Y. Qiu, J. Yu, J. Sun, X. Fan, and G. Yu, "RMC – A Monte Carlo code for reactor core analysis," *Annals of Nuclear Energy*, vol. 82, pp. 121–129, 2015. Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013, SNA + MC 2013. Pluri- and Trans-disciplinarity, Towards New Modeling and Numerical Simulation Paradigms.

[10] T. M. Pandya, S. R. Johnson, T. M. Evans, G. G. Davidson, S. P. Hamilton, and A. T. Godfrey, "Implementation, capabilities, and benchmarking of Shift, a massively parallel Monte Carlo radiation transport code," *Journal of Computational Physics*, vol. 308, pp. 239–272, 2016.

[11] E. Teuchert et al., "V.S.O.P ('94) Computer Code System for Reactor Physics and Fuel Cycle Simulation," Research Report Jülich-2897, Forschungszentrum Jülich, 1994.

[12] H. D. Gougar, A. M. Ougouag, W. K. Terry, and K. N. Ivanov, "Automated design and optimization of pebble-bed reactor cores," *Nuclear Science and Engineering*, vol. 165, no. 3, pp. 245–269, 2010.

[13] D. She, Z. Liu, J. Guo, and L. Shi, "Leakage correction in group-constant generation for pebble-bed HTGRs," *Progress in Nuclear Energy*, vol. 105, pp. 76–82, 2018.

[14] Hans D. Gougar and Abderrafi M. Ougouag and Javier Ortensi and Cristian Rabiti, "Suitability of energy group structures commonly used in pebble bed reactor core diffusion analysis as indicated by agreement with transport theory for selected spectral indices," in *Proceedings of HTR 2018*, (Warsaw, Poland), October 8-10 2018.

[15] V. K. . R. Sanchez, "Core homogenization method for pebble bed reactors," in *M&C 2005: international topical meeting on mathematics and computation, supercomputing, reactor physics and nuclear and biological applications*, (France), 2005.

[16] M. Grimod, R. Sanchez, and F. Damian, "A dynamic homogenization model for pebble bed reactors," *Journal of Nuclear Science and Technology*, vol. 52, no. 7-8, pp. 932–944, 2015.

[17] Q. Wang, D. She, B. Xia, and L. Shi, "Evaluation of pebble-bed homogenized cross sections in HTGR fuel cycle simulations," *Progress in Nuclear Energy*, vol. 117, p. 103041, 2019.

[18] F. Vitullo, J. Krepel, J. Kalilainen, H. Prasser, and A. Pautz, "Statistical Burnup Distribution of Moving Pebbles in the High-Temperature Reactor HTR-PM," *ASME J of Nuclear Rad Sci.*, vol. 6(2), 2 2020.

[19] Sebastian Schunert and Guillaume Giudicelli and Alexander Lindsay and Paolo Balestra and Sterling Harper and Ramiro Freile and Mauricio Tano and Jean Ragusa, "Deployment of the Finite Volume Method in Pronghorn for Gas- and Salt-Cooled Pebble-Bed Reactors," Research Report INL/EXT-21-63189, Idaho National Laboratory, 2021.

[20] A. Hébert, *Applied reactor physics*. Presses inter Polytechnique, 2009.

[21] Z. L. et al., "Cumulative migration method for computing rigorous diffusion coefficients and transport cross sections from Monte Carlo," *Annals of Nuclear Energy*, vol. 112, p. 507–516, 2018.

[22] A.J. Novak and S. Schunert and R.W. Carlsen and P. Balestra and D. Andrs and J. Kelly and R.N. Slaybaugh and R.C. Martineau, "Pronghorn Theory Manual," Research Report INL/EXT-18-44453-Rev1, Idaho National Laboratory, 2020.

[23] , "Benchmark of the Modular High-Temperature Gas-Cooled Reactor (MHTGR)-350 MW Core Design," Technical Report NEA/NSC/R(2017)4, OECD/NEA, February 2018.

[24] B. Hürttlen, W. Meuthen, H. Nabielek, G. Pott, F. Putsch, and F. Schmidt, "Irradiation testing in the jülich research reactor DiDO," tech. rep., 1989.

[25] A. E. Slaughter and Z. M. Prince, "Moose modules: stochastic tools user manual," 2020.

[26] P. Balestra, S. Schunert, R. W. Carlsen, A. J. Novak, M. D. DeHart, and R. C. Martineau, "Pbmr-400 benchmark solution of exercise 1 and 2 using the moose based applications: Mammoth, pronghorn," in *EPJ Web of Conferences*, vol. 247, p. 06020, EDP Sciences, 2021.

[27] A. Novak, J. Peterson, L. Zou, D. Andrš, R. Slaybaugh, and R. Martineau, "Validation of pronghorn friction-dominated porous media thermal-hydraulics model with the sana experiments," *Nuclear Engineering and Design*, vol. 350, pp. 182–194, 2019.

[28] J. Lee, P. Balestra, S. Schunert, A. Novak, Y. Hassan, M. DeHart, and R. Martineau, "Pronghorn fully compressible equation set validation against sana open plenum experiments," *Proc. HTR*, 2020.

[29] Y. Zheng, L. Shi, and Y. Dong, "Thermohydraulic transient studies of the Chinese 200MWe HTR-PM for loss of forced cooling accidents," *Annals of Nuclear Energy*, vol. 36, no. 6, pp. 742–751, 2009.

[30] D. Brown, M. Chadwick, R. Capote, A. Kahler, A. Trkov, M. Herman, A. Sonzogni, Y. Danon, A. Carlson, M. Dunn, D. Smith, G. Hale, G. Arbanas, R. Arcilla, C. Bates, B. Beck, B. Becker, F. Brown, R. Casperson, J. Conlin, D. Cullen, M.-A. Descalle, R. Firestone, T. Gaines, K. Guber, A. Hawari, J. Holmes, T. Johnson, T. Kawano, B. Kiedrowski, A. Koning, S. Kopecky, L. Leal, J. Lestone, C. Lubitz, J. Márquez Damián, C. Mattoon, E. McCutchan, S. Mughabghab, P. Navratil, D. Neudecker, G. Nobre, G. Noguere, M. Paris, M. Pigni, A. Plompen, B. Pritychenko, V. Pronyaev, D. Roubtsov, D. Rochman, P. Romano, P. Schillebeeckx, S. Simakov, M. Sin, I. Sirakov, B. Sleaford, V. Sobes, E. Soukhovitskii, I. Stetcu, P. Talou, I. Thompson, S. van der Marck, L. Welser-Sherrill, D. Wiarda, M. White, J. Wormald, R. Wright, M. Zerkle, G. Žerovnik, and Y. Zhu, "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," *Nuclear Data Sheets*, vol. 148, pp. 1–142, 2018. Special Issue on Nuclear Reaction Data.