



# Evaluation of Dragon's different Self-shielding Calculations Methods using MCNP monte carlo code: Case study: Unit II BNPP Fuel

Kamal Hadad<sup>1\*</sup>, Sajjad Hassanpour<sup>1</sup>

<sup>1</sup>Department of Nuclear Engineering, school of Mechanical Engineering, Shiraz university, Shiraz 71936-16548, Shiraz, Iran

\* Email: kamal.hadad@gmail.com

#### Abstract

Many calculation in the reactor core requires solving the Boltzmann neutron transport equation, which due to the complexity of this equation, numerical methods are used to solve it. Results of numerical solution can be trusted when corrections of the resonance self-shielding effect (Which is just one of the effective parameters) are included and new cross sections are obtained. These corrections can be made by a method called the subgroup method and can be done through deterministic code such as DRAGON. Therefore, the resonance self-shielding effect calculation has been performed for fuel of unit-2 of Bushehr Nuclear Power Plant and its results have been matched with the results of MCNP code (Although this kind of calculations inherently has a degree of uncertainty).

Keywords: Resonance self-shielding, DRAGON code, MCNP code, Fuel rod

#### Introduction

The neutron transport equation is an integral-differential equation with seven independent variables in terms of time, space, energy and angle. The analytical solution of the neutron transport equation can be easily found for simple problems, but is practically impractical for real problems in reactor core analysis. The 2-step calculations have become conventional in reactor core calculations. In first step, a lattice code, generally a neutron transport algorithm solver, evaluates the effective cross section library based on the detailed core indoemation, In the next step, a core calculation code, usually a neutron diffusion algorithm solver, uses the effective cross section library and evaluates the core's neutronic parameters. Numerical methods have been developed to solve the neutron transport equation, which are generally divided into two stochastic deterministic and methods. computational resources are limited due to the complexity of the equation, it makes sense to try definitive methods based on physical and mathematical approximations to reduce the complexity of highdimensional phase space as well as to provide accurate results in a computational time [1]. Neutron flux and cross-sectional calculations require resonance selfshielding calculations to determine the correct amount values of neutron cross sections of the core [2]. With the start of construction of unit-2 of Bushehr Nuclear Power Plant, This research independently to assess core calculations with different resonance self-shielding methods to achive the optimized cross section library for the reactor core. The presence of Gadolinium isotopes in unit-2 fuel (TVS-2M type), and its low energy resonances makes the resonance self shielding calcualtions become more important for creating a reliable cross section library.

DRAGON code with WIMS libraries is well documented and validated deterministic computational codes to perform lattice computation [3, 4]. Dragon provides advanced methods for resonance self-shielding calculations including Generalized Stamm'ler model, subgroup and Tone methods [5, 6].

In this paper we present the results of performing resonance self-shielding calculations for unit-2 BNPP fuel pins, different methods provided by using the Dragon Code. The results are compred with MCNP monte carlo to assess the appropriate self shilding method for BNPP-II core library preparation.

In 2018, Alain used a new method for resonance self-shielding calculations called the Tone method, which is based on Heterogeneous-Homogeneous equivalence principle [7].

In 2017, Palma et al. calculated the neutron flux as relative and absolute using the activation method. However, using this technique to determine the resonance self-shielding factors in the epidermal (middle) range requires knowledge of the Doppler phenomenon [8].

In 2015, Yuxuan Liu in his dissertation reviewed three common methods for performing resonance self-shielding calculations, which he simulated with different software, and then listed the advantages and





disadvantages of each method. For example, two of these three methods, when combining materials (MOX fuel or Gd fuel), can not accurately model the resonance interference, which of course is not very significant for fresh fuel materials, so overall the results Acceptable was obtained [1].

In 2004, Alpan et al. Performed resonance self-shielding calculations for the core with  $UO_2$  fuel as well as for the uranium-238 isotope using the Bondarenko method, and then compared it with two other methods, including the subgroup method. The subgroup method has less error than other resonance self-shielding methods [9].

In 1994, Hogenbirk investigated resonance self-shielding calculations using the MCNP code using the NJOY cross-sectional library. Finally, he observed that this phenomenon has a great effect on the neutron flux in the mid-energy region [10].

In 2020, Xiao et al. Validate the TRX and BAPL criteria between the ENDF / B-VIII.0 and ENDF / B-VIII.0 libraries using the code DRAGON5.0.6 with 281 WIMS-D groups and a library DRAG and compared with Monte Carlo code and experimental values. In order to confirm the DRAGON code, the effect of resonance self-shielding method and leakage model were investigated in this paper. Finally, the results showed that the use of resonance self-protection method in TRX and BAPL criteria is more accurate [11].

In 2017, Hébert et al. calculated the International Atomic Energy Agency benchmark for nuclear fuel management validation for WWERs (IAEA-TECDOC-847) using the Version5 code system (DRAGON and DONJON). These calculations were performed for VVER-1000 reactors while performing cardiac calculations with DRAGON and creating a multivariate cross-sectional database for the main computations with DRAGON. However, resonance self-shielding calculations were also used to perform this process, which increased the accuracy of the calculations [12].

In 2007, Hébert explored techniques and methods that could be used to illustrate the phenomenon of resonance self-shielding in reactor calculations using DRAGON code [13].

Figure 1 shows the graph of neutron interaction with U238 versus neutron energy. from about 1 eV to 100 KeV, the cross-sectional area varies greatly [1].

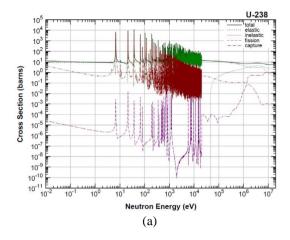


Figure 1. Neutron cross-sectional changes with energy for Uranium-238

### Experimental

#### Preparation of the materials

The fuel assemblies of unit-2 of Bushehr Nuclear Power Plant (BNPP-II) known as TVS-2M, contain both  $UO_2$  fuel pellets as well as  $UO_2 + Gd_2O_3$ . Table 1 presents isotope composition of 2 and 3.6 percent enriched fuels.

**Table 1.** Weight fraction of isotopes in two types of fuel rods of BNPP-II<sup>1</sup>

Weight fraction	% enrichment with gadlenium oxide		% enrichment without gadlenium oxide				
Materials	2% UO <sub>2</sub> + 8% Gd <sub>2</sub> O <sub>3</sub>	3.6% UO <sub>2</sub> + 5% Gd <sub>2</sub> O <sub>3</sub>	2% UO <sub>2</sub>	3.6% UO <sub>2</sub>			
		Mix 1					
O 16	0.11961	0.11259	0.11850	0.11852			
U 235	0.01601	0.02977	0.01741	0.03134			
U 238	0.79495	0.80762	0.86408	0.85012			
Gd 152	0.00013	0.00013	-	-			
Gd 154	0.00149	0.00149	-	-			
Gd 155	0.01022	0.01022	-	-			
Gd 156	0.01420	0.01420	-	-			
Gd 157	0.01088	0.01088	-	-			
Gd 158	0.01726	0.01726	-	-			
Gd 160	0.01520	0.01520	-	-			
		Mix 2					
Hf 72	0.00030	0.00030	0.00030	0.00030			
Zr 90	0.50979	0.50979	0.50979	0.50979			
Zr 91	0.11086	0.11086	0.11086	0.11086			
Zr 92	0.16927	0.16927	0.16927	0.16927			
Zr 94	0.17224	0.17224	0.17224	0.17224			
Zr 96	0.02771	0.02771	0.02771	0.02771			
Nb 93	0.01000	0.01000	0.01000	0.01000			
Mix 3							
H 1	0.11140	0.11140	0.11140	0.11140			
O 16	0.88752	0.88752	0.88752	0.88752			
B 10	0.00019	0.00019	0.00019	0.00019			
B 11	0.00087	0.00087	0.00087	0.00087			
He 4	1.00000	Mix 4 1.00000	1.00000	1.00000			

<sup>&</sup>lt;sup>1</sup> This table does not include all the enrichments.





The presence of  $Gd_2O_3$  has led to the elimination of burnable absorber in the design of the fuel assembly and the emergence of a new form of resonance self-shielding effect in fuel rods. In the presence of  $Gd_2O_3$ , energy self-shielding overcomes spatial self-shielding and makes its distinct from the previous calculations [14]. Since MCNP corrects the resonance self-shielding effect automatically and is a probabilistic and accurate code, its results can be used to validate the our deterministic calculations [10]. The simulated geometry for the unit-2 fuel rod can be seen in Figures 2 and 3.

Dragon provides three modules of USS, SHI and TONE that allows the self-shielding effect calculations. USS is Module for subgroup method, SHI is Module for Stamm'ler method And TONE is based on Heterogeneous-Homogeneous equivalence principle, is Module for Tone method [15].

Therefore, using Table 2 and also using USS, SHI and TONE modules, we perform our calculations in three steps.

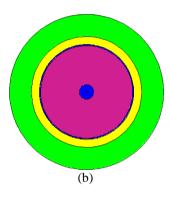


Figure 2. Sectional cutting of the fuel rod of unit-2 simulated in vised<sup>1</sup> software

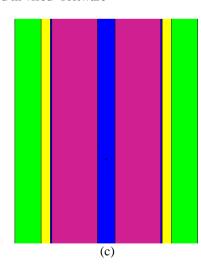


Figure 3. Transverse cutting of the fuel rod of unit-2 simulated in vised software

#### Results

The fuel rods of unit-2 of Bushehr Nuclear Power Plant are simulated in DRAGON and MCNP codes, the results of which can be seen in Table 2. These results are calculated in the form of the effective multiplication factor, which is very important in the reactor core.

**Table 2.** Results obtained from simulation of fuel rods of of BNPP-II<sup>2</sup>

K-eff	% enrichment with gadlenium oxide		% enrichment without gadlenium oxide	
Type of code	2% UO <sub>2</sub> + 8% Gd <sub>2</sub> O <sub>3</sub>	3.6% UO <sub>2</sub> + 5% Gd <sub>2</sub> O <sub>3</sub>	2% UO <sub>2</sub>	3.6% UO <sub>2</sub>
				,
MCNP	0.18280	0.30279	1.11564	1.28065
standard deviation	0.00041	0.00056	0.00248	0.00233
DRAGON (USS) Subgroup method	0.156554	0.266559	1.016477	1.208669
DRAGON (SHI) Stamm'ler method	0.156523	0.266002	1.017068	1.208886
DRAGON (TONE) Tone method	0.155241	0.263375	1.003054	1.192614

The numbers obtained in this simulation are categorized and summarized for better comparison in Figure 4. The horizontal axis represents the percentage of enrichment.

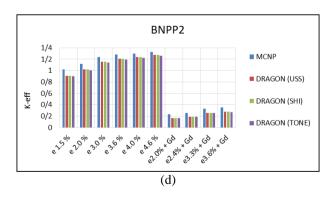


Figure 4. Comparison of the results obtained from the simulation of fuel rods of unit-2 of Bushehr Nuclear Power Plant

<sup>&</sup>lt;sup>1</sup> The Visual Editor for MCNP.

<sup>&</sup>lt;sup>2</sup> This table does not have all the enrichments. The results of other enrichments are shown in Figure 4.





#### Discussion

By looking at the simulation results with MCNP and DRAGON codes, we will find the accuracy of this data and also find the best way to perform resonance shield calculations. By executing both codes with the same MCNP code inputs, the accuracy of DRAGON results can be checked or even fixed. As shown in Figure 4, the distance between the results is very small. To the extent that this difference can be ignored. However, it is clear that with increasing uranium enrichment, the amount of effective multiplication factor also increases and naturally the difference in results also increases slightly. The source of this discrepancy can be found in the details of the geometry as well as the libraries used in the two codes.

The cross-sectional library of both codes is derived from the ENDF reference core data. The NJOY code is generated by the ENDF processing of the library in ACER format, which is the cross-section of a relatively continuous function of energy. The same WIMS library code creates a discrete energy structure for DRAGON. Therefore, the difference in libraries is due to their energy structure, which can cause differences in the results of these two codes.

If we look closely at the figures and tables, we find that not only is there no significant difference between the two subgroup and Stamm'ler methods, but even at low enrichments, the numbers are quite similar. The results in these two methods are very similar to the MCNP results and have very good accuracy. However, in high enrichment, the results of the subgroup method are more accurate and closer to the reference data. A more complete comparison between the self-shielding computational methods is given in the attached references [1,2]. But in the new method called TONE method, the obtained results are more different from other results. As uranium enrichment increases, this difference becomes more acute and further away from the main results.

With increasing energy, the Stamm'ler method is closer to Monte Carlo than other methods.

As we can see in Table 3, the difference between the results of Dragon modules and MCNP is very small. We explained the reasons.

**Table 3.** Comparison of simulation results with Dragon and MCNP

Differences between K-eff	% enrichment with gadlenium oxide		% enrichment without gadlenium oxide	
Type of code	2% UO <sub>2</sub> + 8% Gd <sub>2</sub> O <sub>3</sub>	3.6% UO <sub>2</sub> + 5% Gd <sub>2</sub> O <sub>3</sub>	2% UO <sub>2</sub>	3.6% UO <sub>2</sub>
MCNP and DRG(USS)	0.026246	0.036231	0.099163	0.071981
% Diff.	16.76%	13.59%	9.7%	5.8 %
MCNP and DRG(SHI)	0.026277	0.036788	0.098572	0.071764
% Diff.	16.78%	13.82%	9.6%	5.9%
MCNP and DRG(Tone)	0.027559	0.039415	0.112586	0.088036
% Diff.	17.75%	14.96%	11.22%	7.3%
DRG(USS) and DRG(SHI)	0.000031	0.000557	0.000591	0.000217
% Diff.	0.019%	0.20%	0.058%	0.017%
DRG(USS) and DRG(Tone)	0.001313	0.003184	0.013423	0.016055
% Diff.	0.84%	1.2%	1.3%	1.3%
DRG(SHI) and DRG(Tone)	0.001282	0.002627	0.014014	0.016272
% Diff.	0.82%	0.99%	1.3%	1.3%

### Conclusions

Subgroup method in DRAGON code is the best and closest method to Monte Carlo for calculating the resonance self-shielding effect, which performs cross-sectional corrections correctly. Through this method, both energy self- shielding and spatial self- shielding are considered. However, other methods are also useful and practical.

The BNPP-II fuel assembly uses  $Gd_2O_3$  fuel rods that require resonanse self-shielding corrections. Stamm'lers method also has a good approximation to Monte Carlo. The results of this method are very close to the subgroup method. The Tone method has been traditionally applied to fast reactor analysis with fine or ultrafine group energy mesh. The use of this method is not recommended at high energies and high enrichments.

The subgroup method has disadvantages, especially for the fuel clad, which is not seen in the Stamm'ler and Tone method, and can be filled by presenting a new method that combines all three methods. That will be of future plans.





Acknowledgments

The authors thank Proff. Alain Hébert (Department of Mechanical Engineering, Polytechnique Montréal University, Montréal, Canada) and Proff. Guy Marleau (Department of Mechanical Engineering, Polytechnique Montréal University, Montréal, Canada) for providing technical supports.

### References

- [1] Yuxuan Liu. (2015). A Full Core Resonance Selfshielding Method Accounting for Temperaturedependent Fuel Subregions and Resonance Interference. a dissertation for the degree of Doctor of Philosophy, University of Michigan.
- [2] Jessee, M. A., et al. (2021). Lattice physics calculations using the embedded self-shielding method in Polaris, Part I: Methods and implementation. *Annals of Nuclear Energy*, 150, 107830.
  - https://doi.org/10.1016/j.anucene.2020.107830
- [3] Kromar, M., & Kurinčič, B. (2012). DRAGON and CORD-2 nuclear calculation of the NPP Krško fuel assembly. *Nuclear Engineering and Design*, 246, 58–62.
  - https://doi.org/10.1016/j.nucengdes.2011.06.043
- [4] Martin, N., Hébert, A., & Marleau, G. (2010). DRAGON solutions to the 3D transport benchmark over a range in parameter space. *Annals of Nuclear Energy*, 37(8), 1107–1114. https://doi.org/10.1016/j.anucene.2010.04.003
- [5] Foad, B., & Refeat, R. (2018). Estimation of resonance self-shielding effect in PWR pin cell for different fuel types. *Annals of Nuclear Energy*, 120, 805–813.
  - https://doi.org/10.1016/j.anucene.2018.06.045
- [6] Karthikeyan, R., & Hébert, A. (2008). Performance of advanced self-shielding models in DRAGON Version4 on analysis of a high conversion light water reactor lattice. *Annals of Nuclear Energy*, 35(5), 963–975.
  - https://doi.org/10.1016/j.anucene.2007.09.005
- [7] Alain, H. (2018). an Investigation of Distributed Self-Shielding Effects With the Tone 'S Method. PHYSOR 2018: Reactor Physics Paving The Way Towards More Efficient Systems, April, 1490–1502
- [8] Palma, D. A. P., Almeida, G. G., & Gonçalves, A. C. (2017). Calculation of resonance self-shielding factors in a round disk using the enlarged Doppler Broadening Function. *Annals of Nuclear Energy*, 109, 380–384.
  - https://doi.org/10.1016/j.anucene.2017.05.051
- [9] Alpan, F. A., Leal, L. C., & Courcelle, A. (2004). Effect of energy self-shielding methods on 238U for criticality safety problems. Proceedings of the PHYSOR 2004: The Physics of Fuel Cycles and Advanced Nuclear Systems - Global

- Developments, 2004, 2209-2218.
- [10] Hogenbirk, A. (1994). Why self-shielding is needed in MCNP calculations. *Symposium of Fusion Technology, September*.
- [11] Xiao, et al. (2020). Critical verification for TRX and BAPL benchmarks based on ENDF/B-VIII.0 using DRAGON code. *Annals of Nuclear Energy*, *146*, 107661. https://doi.org/10.1016/j.anucene.2020.107661
- [12] Hébert, A., et al. (2017). Analysis of a VVER-1000 in-core fuel management benchmark with DRAGON and DONJON. *International Journal*

of Nuclear Energy Science and Technology, 11(4),

345. https://doi.org/10.1504/ijnest.2017.10011836

- [13] Hébert, A. (2007). A review of legacy and advanced self-shielding models for lattice calculations. *Nuclear Science and Engineering*, 155(2), 310–320.
  - https://doi.org/10.13182/NSE06-50
- [14] Ghaemi, S., & Faghihi, F. (2021). Core designing of a new type of TVS-2M FAs: neutronics and thermal-hydraulics design basis limits. *Frontiers in Energy*, *15*(1), 256–278. https://doi.org/10.1007/s11708-018-0583-x
- [15] Arleau, G. M. (2013). A User Guide for DRAGON. 12(July), 1–15.