VNU Journal of Science: Mathematics – Physics, Vol. 36, No. 4 (2020) 66-75

VNU Journal of Science: Mathematics - Physics

Journal homepage: https://js.vnu.edu.vn/MaP

Original Article

Comparison of Deterministic and Stochastic Depletions in Graphite-Filled MOX Fuel Assembly Design

Thanh Mai Vu[1,*], Donny Hartanto[2]

[1]*Faculty of Physics, VNU University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam*

[2]*Department of Mechanical and Nuclear Engineering, University of Sharjah, P.O.BOX, 27272, Sharjah, United Arab Emirates*

Received 08 April 2020
Revised 22 May 2020; Accepted 09 June 2020

Abstract: A comparison between stochastic and deterministic depletion calculations based on a graphite-filled MOX fuel assembly configuration is presented in this paper. The infinite multiplication factors and isotope inventory changes as a function of burnup obtained by Monte Carlo method module SCALE/KENO and deterministic method module SCALE/NEWT are compared with those obtained by deterministic code HELIOS. The impact in calculation results by using different nuclear data library is also investigated. The SCALE/KENO results show a good agreement with SCALE/NEWT results in the eigenvalue as a function of burnup (less than 0.1%). However, the absolute difference in the initial k_∞ between SCALE/KENO and NEWT modules and HELIOS results is quite large (around 1.1%) and the isotope inventory changes show quite differently at the end of cycle. The uranium and plutonium depletion rates calculated by SCALE/KENO and SCALE/NEWT have quite good agreement. By using the same data library, the good agreement between stochastic and deterministic code's results were confirmed.

Keywords: Monte Carlo method, deterministic method, reactivity calculation, inventory changes.

1. Introduction

While producing energy, a nuclear power plant also produces plutonium and other heavy metals from the neutron capture of U^{238}. The produced plutonium can be recycled and used again as a nuclear fuel. From the spent nuclear fuel, the remained uranium and the produced plutonium are recovered

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*Corresponding author.
Email address: mai_vu@hus.edu.vn

https//doi.org/ 10.25073/2588-1124/vnumap.4499

through chemical recycling process. The recovered uranium and plutonium are then used to fabricate mixed oxide (MOX) fuel. This type of the fuel is now widely use in France and Japan [1]. However, the MOX fuels are loaded into the pressurized water reactor (PWR) core with limited number due to different characteristics than that of the conventional uranium fuel. One of the disadvantages of using MOX fuel is the hardening of the neutron spectrum [2, 3].

In order to overcome the spectrum hardening effect from plutonium isotopes in MOX fuel and to be able to have a core fully loaded with MOX fuels, a minor modification from the conventional 16X16 PWR type fuel assembly was proposed [3]. It is characterized by an internal region of the fuel rod filled with graphite and the proposed fuel assembly design was called gMOX. The burnup performance had been performed using the deterministic code HELIOS [4]. However, the deterministic methods solve the multi-group transport equation to get the average neutron behavior. They have limitations in solving the complex geometry and continuous energy problem. Monte Carlo codes overcome these problems, thus, comparing with deterministic codes, they will have broader applications, and sometimes play a unique role in research [5].

A brief discussion on the characteristics of Monte Carlo and deterministic code that is important for fuel cycle analysis will be presented. The burnup calculation for gMOX fuel assembly is carried out using SCALE module TRITON/KENOV (SCALE/KENO for short) and module TRITON/NEWT (SCALE/NEWT for short) [6] to compare with HELIOS result in terms of multiplication factor as a function of burnup. Although plutonium isotopes were shown to be depleted more in gMOX fuel than conventional MOX fuel [3], it is important to quantify their detail composition, especially the fissile content, because that will affect both storage and repository designs.

2. Depletion Codes

Two different code systems are chosen this investigation: SCALE (SCALE/KENO module and SCALE/NEWT module) and HELIOS code. They are markedly different in both methods and data used. Descriptions of each code and sources of their nuclear data are given below.

2.1. SCALE

In SCALE code, TRITON serves as the controller of module sequencing, data transfer, and input/output control for multiple analysis sequences. Resonance cross section is processed due to BONAMI/CENTRM/PCM functions. To calculate the multiplication factor and fluxes, SCALE can support for both stochastic and deterministic methods. For stochastic calculation, TRITON calls KENOV, a Monte Carlo code that calculates multiplication factor for three-dimensional system. In order to obtain keff and fluxes using deterministic method, NEWT code is used as the part of SCALE sequence. NEWT code is a multi-group discrete ordinates transport code with flexible meshing capabilities that allow two-dimensional neutron transport calculations using complex geometric models [6].

ORIGEN-S performs both nuclide generation and depletion calculation for specified burnup steps. Yields are given for 30 fissionable actinides including $Th^{227,228,232}$, Pa^{231}, $U^{232\text{-}238}$, $Pu^{238\text{-}242}$, $Am^{241,242m,243}$, $Np^{237,238}$, $Cm^{242\text{-}246,248}$, $Cf^{249,252}$, Es^{254}. Fission product yield data were acquired primarily from ENDF/B-VI [7]. The predictor–corrector algorithm is applied in TRITON calculation.

For this burnup calculation, SCALE calculation for gMOX fuel assembly was used 238-group ENDF/B-VI based library.

2.2. HELIOS

HELIOS is a current-coupled collision probabilities (CCCP) code which is applied to perform lattice burnup calculation in two-dimensional geometry [4]. In HELIOS, B1 method is employed to evaluate the criticality spectrum of the neutron fluxes and enforces this spectrum on the neutron flux obtained from CCCP method. In contrast to SCALE predictor-corrector algorithm, full-blown predictor–corrector strategy is used to get the new number densities of the individual materials [5].

In study by Jo et al.'s study [3], the burnup calculation for the gMOX fueled assembly was conducted using HELIOS with 89-group ENDF/B.V cross section library which is an older updated version than other depletion code systems using in this study. Therefore, further notice should be spent when comparing the HELIOS results to the other depletion codes results which use different versions of cross section library.

The major factors of each code are summarized in Table 1.

Table 1. Summary of depletion codes

Feature	SCALE/KENO V.a	SCALE/NEWT	HELIOS
Transport treatment	Monte Carlo	Deterministic	
Cross section libraries	ENDF/B-VI	ENDF/B-VI	ENDF/B-V
Number of energy groups	238	238	89
Temperature-dependent cross section	Available	Available	Available
Predictor-corrector algorithm	Halfway	Halfway	Each burnup step
Leakage for spectrum	No	No/B1	No/B1
Actinide representation	129	129	38 (Th^{230} through Cm^{246})
Fission products	1119	1119	115
Fissionable isotopes having explicit fission yields	30	30	28

3. Fuel Assembly Design

To overcome the hardening spectrum effect in MOX fueled assembly, the new fuel design which consists of the annular fuel material filled internally with graphite was proposed and investigated using HELIOS by Jo et al. (Figure 1). From the fuel design modification, higher burnup with less fuel inventory and faster rate of plutonium are obtained [3].

The assembly employs the conventional16X16 PWR type fuel assembly with 236 fuel rods and 5 guide tubes welded to spacer grids (Figure 2). Each guide tube displaces four fuel rod positions. Water which is used as moderator and to fill in guide tube contains 500 ppm of boron.

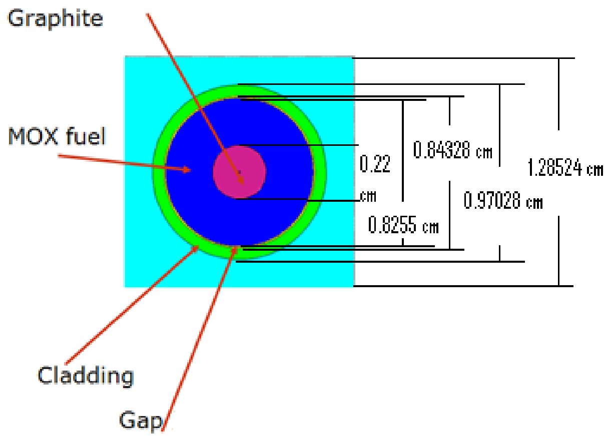

Figure 1. Schematic of cross section of gMOX fuel rod.

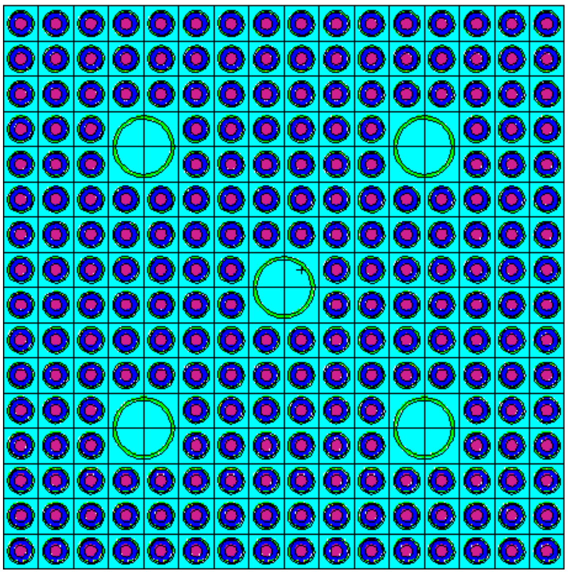

Figure 2. Radial cross section of gMOX fuel assembly

Density of graphite, fuel, gap, cladding and moderator and temperature in each region are shown in Table 2.

Table 2. Material densities and temperatures

Material	**Density (g/cm^3)**	**Temperature (K)**
Graphite	1.6	950
Fuel	10.38	900
Gap	0.001	750
Cladding	6.5	670
Water	0.6974	580

In this work, the depleted uranium (0.225 w/o of U^{235}) is used in the uranium matrix. Total content of plutonium is 5 w/o. The composition of plutonium isotopes is given respectively as Pu^{238}, Pu^{239}, Pu^{240}, Pu^{241}, Pu^{242} and Am^{241} of 1.83, 57.93, 22.50, 11.06, 2.57 and 1.08%. In Table 3, initial fuel number densities are given.

Table 3. Initial fuel number densities

Material	Isotope	Number density (atom/barn-cm)
Graphite	C	8.0293E-02
Fuel	U^{235} U^{238} Pu^{238} Pu^{239} Pu^{240} Pu^{241} Pu^{242} Am^{241} O^{16}	4.94723E-05 2.19382E-02 2.11776E-05 6.70393E-04 2.60380E-04 1.27991E-04 6.48058E-05 1.24983E-05 4.62898E-02
Gap	He^{3} He^{4}	3.9837E-08 2.6799E-02
Cladding	Zr	4.21847E-02
Water	H^{1} O^{16} B^{10} B^{11}	4.6640E-02 2.3320E-02 3.8692E-06 1.5574E-05

4. Results and Discussion

At the first part, the burnup calculation results are obtained using SCALE/KENO and SCALE/NEWT with ENDF/B-VI cross section data without the criticality spectrum calculation. The gMOX fuel undergoes 1200 burnup days with power per assembly is 15.77 MWth and the calculated specified power is 49.3 kWth/kg HM. These results are used to compare with the HELIOS results.

Figure 3 shows the comparison of the multiplication factors as a function of burnup calculated by HELIOS, SCALE/KENO and SCALE/NEWT. As illustrated in the Figure 3, the sharp decrease at the beginning is due to the build-up of xenon and samarium. For more accuracy, small burnup periods should be applied for several initial burnup steps. A large descrepancy (about 1.1%) between initial multiplication factor of SCALE/KENO and SCALE/NEWT and HELIOS calculation was found. The impact of different nuclear data versions (ENDF/B-V used in HELIOS and ENDF/B-VI used in SCALE code) was considered to cause a big discrepancy in reactivity calculation results. The decay scheme and the predictor–corrector method differences cause the bigger discrepancy of k at the end of cycle (EOC). By using the same library version for both stochastic and deterministic codes, the discrepancies between SCALE/KENO and SCALE/NEWT results are much smaller. The discrepancy of initial k_∞ of SCALE/KENO and SCALE/NEWT is less than 0.1% and the discrepancy at burnup 60 GWd/MTU is 0.2%. That shows a reasonable agreement between stochastic and deterministic depletion calculation.

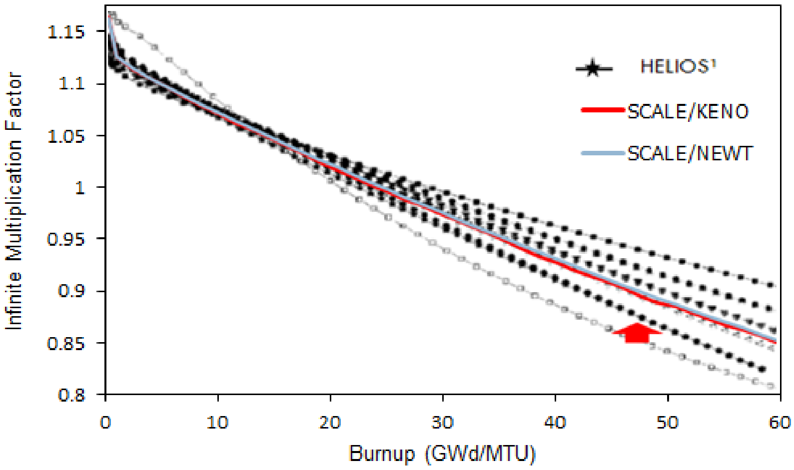

Figure 3. Multiplication factor comparison between HELIOS, SCALE/KENO and SCALE/NEWT.

Important actinides inventories for MOX fuel are shown from Figure 4 to 11. Figure 4 and 5 show a good agreement between deterministic (SCALE/NEWT) and stochastic results (SCALE/KENO) of U^{235} and U^{238} inventory changes. Figure 6 shows a quite big difference in Pu^{238} inventory changes. This difference is accounted for the difference in decay scheme. However, Pu^{238} composition in MOX fuel is so small and does not play an important role in repository criticality concern, the difference between calcuclation code results can be accepted.

The good agreement in the Pu^{239}, Pu^{240}, Pu^{241} and Pu^{242} depletion rates was found for SCALE/KENO and SCALE/NEWT's results (Figure 7, 8, 9 and 10). The differences in those isotopes depletion rates between HELIOS and SCALE codes are larger because of the impact of library version difference.

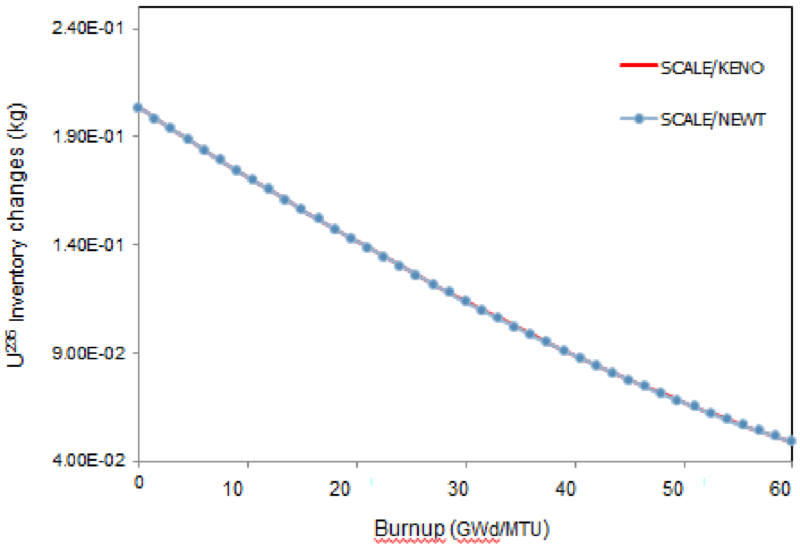

Figure 4. Comparison of inventory changes of U^{235} between SCALE/KENO and SCALE/NEWT.

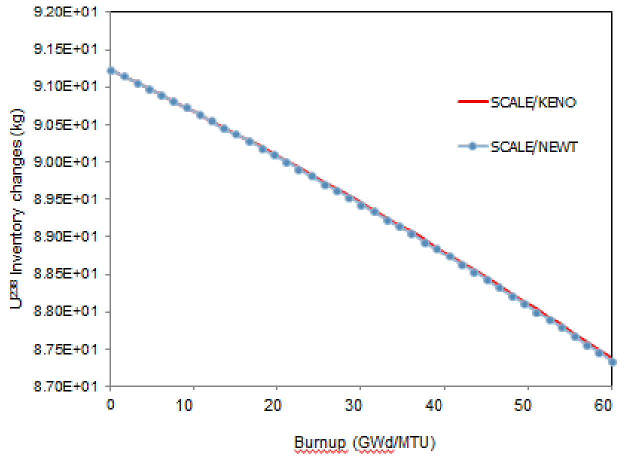

Figure 5. Comparison of inventory changes of U^{238} between SCALE/KENO and SCALE/NEWT.

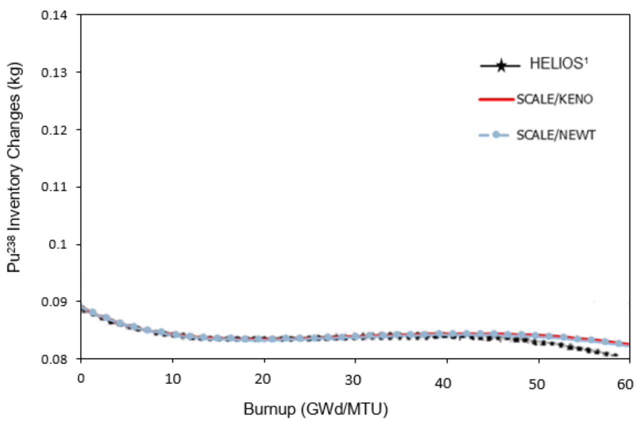

Figure 6. Comparison of inventory changes of Pu^{238} between HELIOS, SCALE/KENO and SCALE/NEWT.

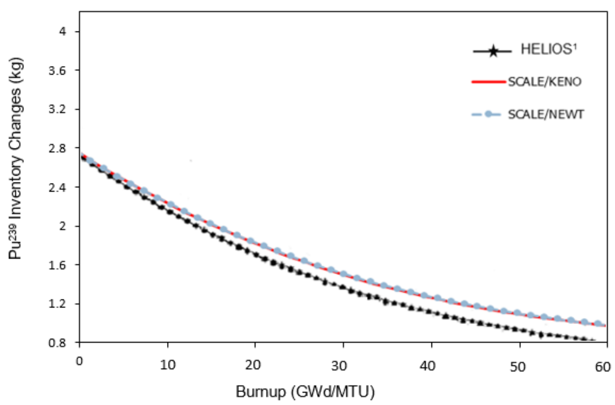

Figure 7. Comparison of inventory changes of Pu^{239} between HELIOS, SCALE/KENO and SCALE/NEWT.

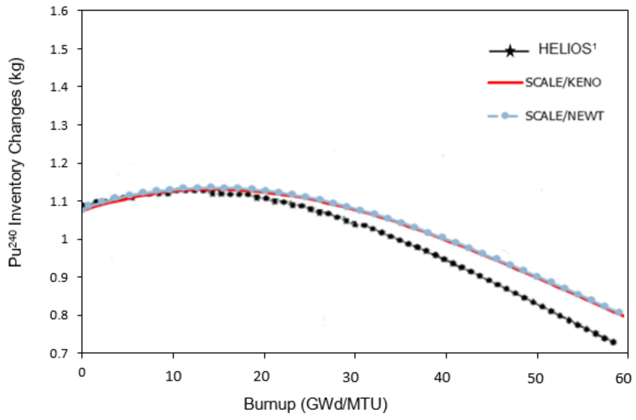

Figure 8. Comparison of inventory changes of Pu^{240} between HELIOS, SCALE/KENO and SCALE/NEWT

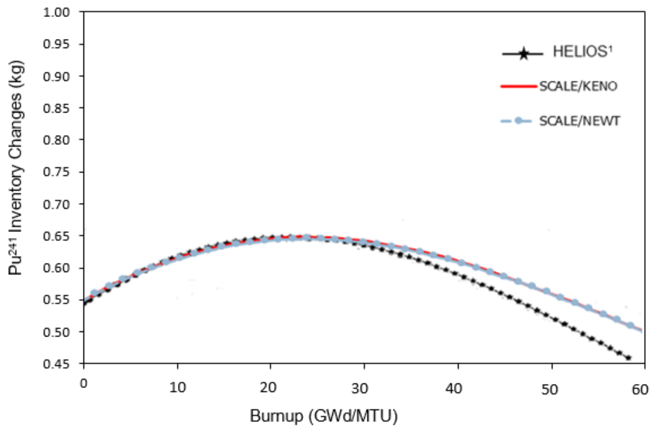

Figure 9. Comparison of inventory changes of Pu^{241} between HELIOS, SCALE/KENO and SCALE/NEWT.

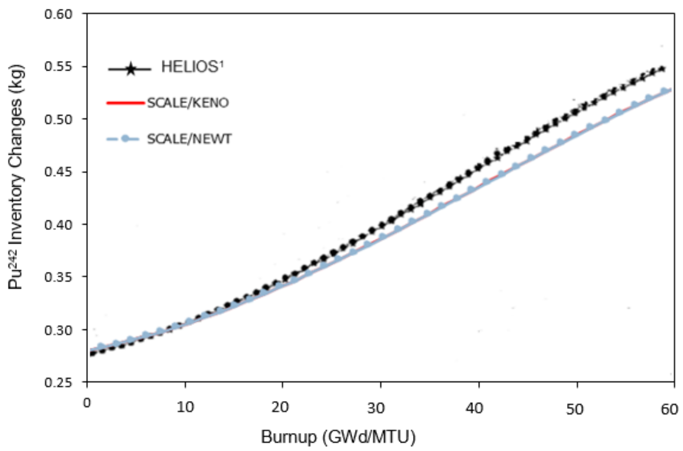

Figure 10. Comparison of inventory changes of Pu242 between HELIOS, SCALE/KENO and SCALE/NEWT.

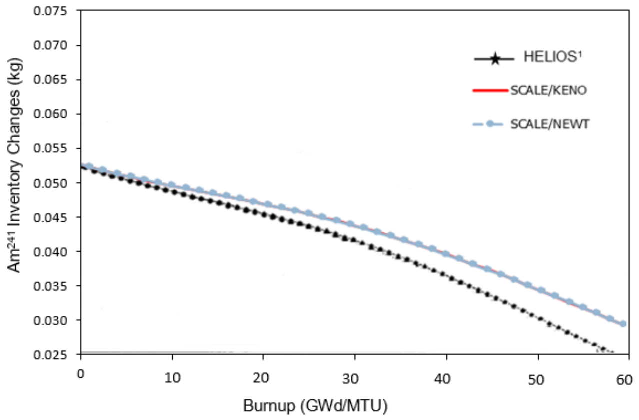

Figure 11. Comparison of inventory changes of Am241 between HELIOS, SCALE/KENO and SCALE/NEWT.

5. Conclusions

In this study, the depletion calculations using Monte Carlo based codes and depletion codes are performed. By using the same cross section library version, ENDF/B-VI, the comparison of eigenvalue as a function of burnup between stochastic depletion, SCALE/KENO and deterministic depletion SCALE/NEWT shows a good agreement. The accuracy of stochastic depletion obtained by SCALE-KENO was verified and can be used in future investigation for gMOX fueled light water reactors. Older library version used in HELIOS leads to relatively large discrepancies compared to other codes. In order to conduct more relevant comparison between calculation results, it is suggested to use same cross section library version. In isotope inventory changes, the results between HELIOS and SCALE show the quite large discrepancy at the end of burnup cycle. The different decay chain and fission isotopes between codes causes the descrepancy in inventory changes of the isotopes after each burnup step and it becomes apart at the end of cycle.

Acknowledgments

This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.04-2019.14. We also would like to thank to Prof. N. Z. Cho (KAIST, Korea) and Dr. C. K. Jo (KAERI) for their great support during this study.

References

[1] International Atomic Energy Agency, Status and Advances in MOX Fuel Technology, Technical Reports Series No. 415, IAEA, Vienna, 2003.

[2] P. Barbrault, A Plutonium-Fueled High-Moderated Pressurized Water Reactor for Next Century, Nuclear Science and Engineering, Vol. 122 (1996), 240-246. https://doi.org/10.13182/NSE96-A24158.

[3] C. K. Jo, N. Z. Cho, and Y. H. Kim, Graphite-Filled Mixed-Oxide Fuel Design for Fully Loaded PWR Cores, Annals of Nuclear Energy 27 (2000) 819-829. https://doi.org/10.1016/S0306-4549(00)00004-9.

[4] J. J. Casal, R. J. J. Stamm'ler, E. A. Villarino, and A. A. Ferri, HELIOS: Geometric Capabilities of a New Fuel-Assembly Program, Proceedings of International Topical Meeting on Advances in Mathematics, Computations and Reactor Physics, Pittsburg, PA, USA, Vol. II, Sect. 10.2.1, 1-13, 1991.

[5] E. E. Lewis and W. F. Miller, Computational Methods of Neutron Transport, American Nuclear Society, 1993.

[6] B. J. Ade, SCALE/TRITON Primer: A Primer for Light Water Reactor Lattice Physics Calculations, NUREG/CR-7041 (ORNL/TM-2011/21), prepared for the U.S. Nuclear Regulatory Commission by Oak Ridge National Laboratory, Oak Ridge, 2012.

[7] Cross Section Evaluation Working Group, ENDF/B-VI Summary Documentation, BNL-NCS-17541 (ENDF-201), Brookhaven National Laboratory, New York, 1996.