EPJ Web of Conferences **308**, 02004 (2024) https://doi.org/10.1051/epjconf/202430802004
ISRD 17

An automated weight window generator based on the recursive Monte-Carlo method for use in MC shielding calculations

Pratibha Yadav[1], *Silvio* Baier[2,*], *Jörg* Konheiser[3], and *Reuven* Rachamin[3]

[1]Technische Universität München, Department of Energy and Process Engineering, Munich, Germany
[2]Technische Universität Dresden, Department of Chemistry and Food Chemistry, Dresden, Germany
[3]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Reactor Safety Division, Dresden, Germany

Abstract. MCNP code provides numerous variance reduction techniques that are mainly used to optimize the analog Monte Carlo simulations. These techniques can reduce the statistical uncertainty of the simulation results while minimizing computational costs. Weight window is one such technique that is commonly used to optimize shielding calculations. However, for complex shielding problems such as deep penetration, the existing MCNP weight window generator is not efficient enough to generate the appropriate weight parameters for the weight window in a single run. To address this issue, an automated algorithm was developed using the code TRAWEI, which is based on recursive Monte Carlo methodology. The TRAWEI code can generate suitable weight values in a single run with less calculation time. This paper focuses on the verification of TRAWEI-generated weights using a simplified cask model. Further, the results of MCNP simulation using TRAWEI-generated weights are compared with those using weights generated by an existing MCNP weight window generator.

1 Introduction

Monte Carlo methods are widely used in the nuclear industry and offer a reliable and precise approach for evaluating the safety of nuclear facilities. These methods, involving Monte Carlo calculations, yield valuable insights in addressing various concerns related to shielding, reactor dosimetry, and activation. MCNP [1] is the established standard code utilized for performing such calculations. In many cases, these calculations frequently encounter deep penetration issues, in which particles travel through thick shield materials to reach regions of interest. As many of the particles are absorbed by the shield materials, problems with deep penetration often result in insufficient particle sampling in the desired region, thus resulting in substantial statistical fluctuations in the analog simulation results. In order to improve the accuracy and efficiency of these simulations, the weight window variance reduction tool is frequently used. In principle, the weight window method aims to

* Corresponding author: s.baier@hzdr.de

improve the sampling of particles by controlling the population of particles entering regions of interest by splitting or Russian roulette [2]. The technique is defined by weight window parameters. Usually, the user utilizes an automated weight window generator embedded within the MCNP code to generate these parameters. This generator produces the weights with the aid of a normal Monte Carlo calculation. However, for complex shielding problems, such as those involving deep penetration, the generator requires multiple iterations to determine the optimal weight window values. Consequently, many users have developed deterministic methods [3, 4, 5] and adaptive methods [6, 7] for effectively producing the weight window values. However, each of these methods has its advantages and limitations. Therefore, the purpose of this study is to establish an automated tool based on recursive Monte Carlo methodology that can generate the optimal set of weight values in a single run with less computational time. The method can be easily integrated into a Monte Carlo code. In this paper, the second section discusses the theoretical basis of the RMC methodology and its implementation in the in-house code TRAWEI [8]. The third section describes the verification of the developed algorithm using a simplified cask model. The conclusion and future prospects are described in the final section.

2 Theory

2.1 Weight window technique

The weight window is a technique that depends on space, energy (or time) and involves splitting or killing particles based on their importance (which is the reciprocal value of their weights) [2]. The user provides a lower weight bound and a width of the weight window for each region or cell. If the weight of a particle exceeds the upper weight bound, it is split such that the splitting particles have a weight within the weight window. Conversely, if the weight of a particle is below the lower weight bound, Russian roulette is played, and the weight of the particle is either increased to be within the weight window or the particle is killed. The weight window generator aims to calculate the importance of each cell by taking into account the expected score that a particle of unit weight would produce at a given location in phase space.

2.2 Recursive Monte Carlo methodology

The recursive Monte Carlo (RMC) method was introduced by Goldstein and Greenspan [9]. We adapted and revised this methodology for the calculation of importance for solving deep penetration problems. In the RMC method, the importance of each cell or region is estimated by solving the forward transport equation and defining the cells one by one as source cells [10]. The calculation commences with the lowest energy group particles for the defined target region and moves towards the next neighbouring region. If a particle reaches the surface of an already estimated importance region, the calculation stops, and the known importance is used to estimate the importance for the preceding calculation. After estimating the importance of all regions with the same energy group, the calculation continues in the same way for the next higher energy group particles. However, during the calculation of higher-energy particles, there is a possibility that the particle may undergo scattering (elastic and inelastic), resulting in its energy falling to the lower energy boundaries. In such instances, the previously estimated importance of lower-energy particles can be used for subsequent calculations. Once the importance is estimated for all regions and for all energy groups, weights are estimated by taking the reciprocal of the importance. This method has the advantage of accelerating weight calculation by utilizing previously estimated importances

from neighboring regions or from lower-energy groups. It is an automated technique that does not require any iterative process.

2.2.1 Mathematical basis of RMC methodology

The fundament of our method is mainly based on the traditional RMC approach of Goldstein and Greenspan [9] and is explained using a simple 2D geometry consisting of nine equal cells, as depicted in Fig. 1. According to Fig. 1, let's assume cell i_3 is the unknown cell, whose importance is to be estimated. Cells i_0, i_1 and i_2, which are shaded in green, represent cells where the importance value is already known. To estimate the importance of cell i_3, we consider i_3, as source cell and start particles randomly distributed in space, direction and energy within the actual energy group. Particles that are reaching the surface S_{13} of the nearest known importance cell i_1 are utilized. Additionally, there is a possibility that particles could reach the surfaces S_{24} and S_{26} of the known importance cell i_2, which can also be used for the importance estimation for the cell i_3.

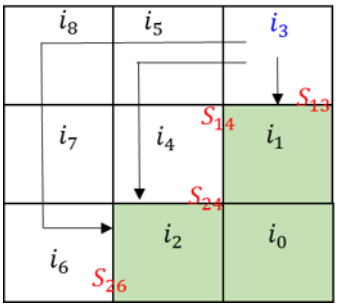

Fig. 1. Schematic illustration of a region divided into sub-regions or cells.

A generalized formulation of RMC has been derived based on the above explanation of RMC working with Fig. 1. Let's define the cells and energy groups by i_m and E_n. Here, m and n are consecutive numbers of cells and energy groups. The surface between cells $i_{m'}$ and $i_{m''}$ is denoted by $S_{m'm''}$. The importance of the target cell i_0 in the lowest energy group E_0 is estimated by equation (1):

$$W(i_0, E_0) = \frac{N_a(i_0, E_0)}{N_s(i_0, E_0)} \tag{1}$$

Here, $N_s(i_0, E_0)$ is the number of source particles within cell i_0 within the energy group E_0. $N_a(i_0, E_0)$ is the number of source particles absorbed within the target cell i_0 within the energy group E_0. Subsequently, for the next neighboring cells i_m, its importance for the same lowest energy group E_0 is estimated by equation (2):

$$W(i_m, E_0) = \frac{1}{N_s(i_m, E_0)} \left(\sum_{m''} \sum_{m'} N(i_m \rightarrow S_{m'm''} | E_0) \times W(i_{m''}, E_0) \right) \tag{2}$$

Here, $N_s(i_m, E_0)$ is the number of source particles within the cell i_m. $N(i_m \rightarrow S_{m'm''}|E_0)$ is the number of particles leaving the current cell via the surface $S_{m'm''}$. $W(i_{m''}, E_0)$ is the known importance value of cell $i_{m''}$. In eq. (2), the summation over m'' represents cells with free surfaces, where the importance is already known, while the summation over m' corresponds to the free surfaces of cell m''. Free surface means a surface between a cell with known importance value and a cell with unknown importance value.
In accordance with the example illustrated in Fig. 1, the summation of m'' corresponds to cells i_1 and i_2, while the summation index m' corresponds to cells i_3 and i_4 for $m'' = i_1$, representing particles that traverse surfaces S_{13} and S_{14}. Similarly, m' corresponds to cells i_4 and i_6 for $m'' = i_2$, which represent particles that traverse surfaces S_{24} and S_{26}.
This is done for all cells within the lowest energy group. Then the procedure is repeated subsequently for all higher energy groups. The calculation of the importance of a higher energy group E_n of the target cell is done by equation (3):

$$W(i_0, E_n) = \frac{1}{N_s(i_0, E_n)} \left(N_a(i_0, E_n) + \sum_{k=0}^{n-1} N_a(E_n \rightarrow E_k|i_0) \times W(i_0, E_k) \right) \tag{3}$$

Here, $N_a(E_n \rightarrow E_k|i_0)$ defines the probability of particles undergoing (elastic or inelastic) scattering with a shift of energy to the lower group E_k. For the next neighboring cells the high energy groups particle importances are estimated by equation (4):

$$W(i_m, E_n) = \frac{1}{N_s(i_m, E_n)} \left(\sum_{m''} \sum_{m'} N(i_m \rightarrow S_{m'm''}|E_n) \times W(i_{m''}, E_n) + \sum_{m'''} \sum_{k=0}^{n-1} N(E_n \rightarrow E_k|i_m \rightarrow i_{m'''}) \times W(i_{m'''}, E_k) \right) \tag{4}$$

The first summand describes the transition of the neutrons to already known regions ($i_{m''}$, staying in the respective energy group E_n), the second summand accounts for the particles that have undergone down scattering to different levels of lower energy groups (e. g., a particle in energy group E_5 may down-scatter to E_4, E_3 or E_2). It also describes down scattering in other cells $i_{m'''}$ (Sum over m''' covers all regions with unknown importance in the actual energy group E_n, including m).

2.2.2 Implementation of RMC using TRAWEI code

The TRAWEI code is used to calculate the weight values necessary for solving particle transport problems (neutrons and gammas). The objective of this code is to estimate the optimal weight values for Monte Carlo calculations in a single step while minimizing computation time. Initially, TRAWEI was developed for the TRAMO code system, which is a specialized Monte Carlo code used for reactor dosimetry and shielding calculations [8, 11]. However, in this study, TRAWEI-generated weights will be used with the reference code MCNP. Before weight estimation, the mesh geometry of a given problem is transferred from

MCNP to TRAWEI. Then, TRAWEI generates a set of appropriate weight values for that problem. After the weights have been determined, they are transferred to MCNP using supported input formats. These weight values are used by MCNP for the actual calculations.

3 Verification of the methodology

3.1 Geometrical description of the test problem

The effectiveness of the TRAWEI-generated weight values has been tested initially with a single shield material problem. It has been proven the functionality of the RMC methodology [10]. In order to test the performance of the TRAWEI-generated weights for a real case problem, a simplified cask model has been prepared that is based on the CASTOR V/19 model [12]. Such cask geometries are commonly used for storing and transporting spent fuel assemblies from pressurized water reactors (PWR). The model includes a spent fuel region, an iron wall, a moderator, and air. It has dimensions of 5.95m in height, 1.4m in inner diameter, and 0.5m in outer diameter. The cask has a moderator layer measuring 11cm in thickness, and an additional two moderator layers measuring 9cm in thickness are placed on the top and bottom of the cask, as illustrated in Fig. 2, where the iron wall is composed of spheroidal graphite cast iron with a density of 7.20g/cm^3, the moderator is made of polyethylene with a density of 0.93g/cm^3. The outside of the cask was assumed to be filled with air, with a density of 1.205mg/cm^3.

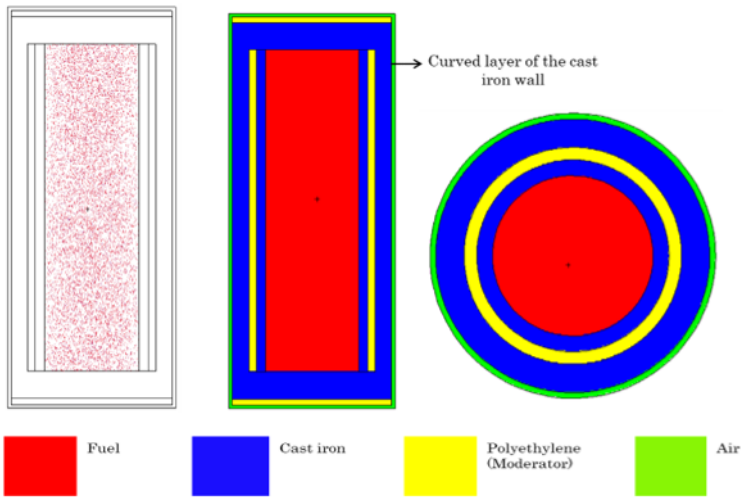

Fig. 2. Schematic view of the simplified cask model.

It has been considered that the fuel source had a homogeneous distribution. The model is utilized to calculate the neutron fluence over the outer cylinder surface of the cast iron wall. To estimate the fluence, three independent calculations were performed, including an analog MCNP simulation without weight window (WW), a simulation using weight parameters generated by the in-built MCNP weight window generator (MCNP-WWG), and a simulation using weight parameters generated by the TRAWEI (RMC) code. The number of neutron particles in each simulation was chosen such that all simulations require roughly the same amount of computer time.

3.1.1 Neutron fluence over the cast iron wall

MCNP weight window generator (MCNP-WWG) and TRAWEI specifically optimized weight values over the outer wall of the cask (cf. Fig. 2). However, with MCNP-WWG, the generated weight values for the actual model were not appropriate as many of the values were zeros, so the reduced density method [7] was used with the MCNP-WWG. It took a total of six iterations, lasting around 70min in total, to generate the optimal weight values using this method. The left column of Fig. 3 shows the fluence distribution obtained from different simulations over the outer wall, which is approximately identical over a large range of orders of magnitude. The right column of Fig. 3 shows the relative error distribution over the outer wall. Compared to the analog MCNP results, both the MCNP results obtained using weight values generated by MCNP-WWG (MCNP-WWs) and the TRAWEI-generated weights (TRAWEI-WWs) yielded a considerably reduced relative error, as shown in the right column of Fig. 3. Notably, the TRAWEI weights produced the most accurate results with the smallest error. Table 1 provides a comparison of the calculation efficiency of the different simulations, which is evaluated in terms of the FOM. The FOM is defined by equation (5):

$$FOM = \frac{1}{Re^2 \times T} \tag{5}$$

Here, Re is the relative error and T is the total time taken by the simulation. It has been observed that overall, the FOM of TRAWEI-WWs is increased compared to the analog MCNP and MCNP-WWs (see the FOM column in Table 1).

Table 1. Comparison of FOM.

Simulation	Computational time (min)			Avg. fluence(n/cm^2 prim-n)	Avg. rel. err.	FOM (1/min)
	WW generation	Tally estimation	Total time			
Analog MCNP	-	103	103	6.6635E-06	0.1122	0.77
MCNP-WWs	70	42	112	6.7356E-06	0.0695	1.85
TRAWEI-WWs	80	21	101	6.6580E-06	0.0584	2.90
Note: FOM has been estimated with the total time.						

4 Conclusion

The weight window method is a popular variance reduction technique used for optimizing Monte Carlo shielding calculations. This method typically requires appropriate weight window parameters to be defined, which can be specified manually or generated by a weight-window generator (WWG) such in MCNP available. However, in cases of complex shielding issues like deep penetration problems, the MCNP weight window generator may reach its statistical limits and require multiple iterations or adapted strategies to produce an appropriate set of weight values, which can be time-consuming and require much user experience. To address this, the present study focuses on using the in-house TRAWEI code, based on the recursive Monte Carlo (RMC) method, to generate optimal weight parameters. To verify the performance of the RMC-based TRAWEI code, several test cases were conducted. Two of these test cases were previously presented in [10], while a new test case focusing on a simplified barrel model is introduced in this paper. The results show that the MCNP calculation using TRAWEI-generated weights uniformly reduced the relative error over the

wall, with an improved figure of merit (FOM) compared to the analog MCNP and the MCNP calculation using MCNP-WWG generated weights. Thus, it can be concluded that the

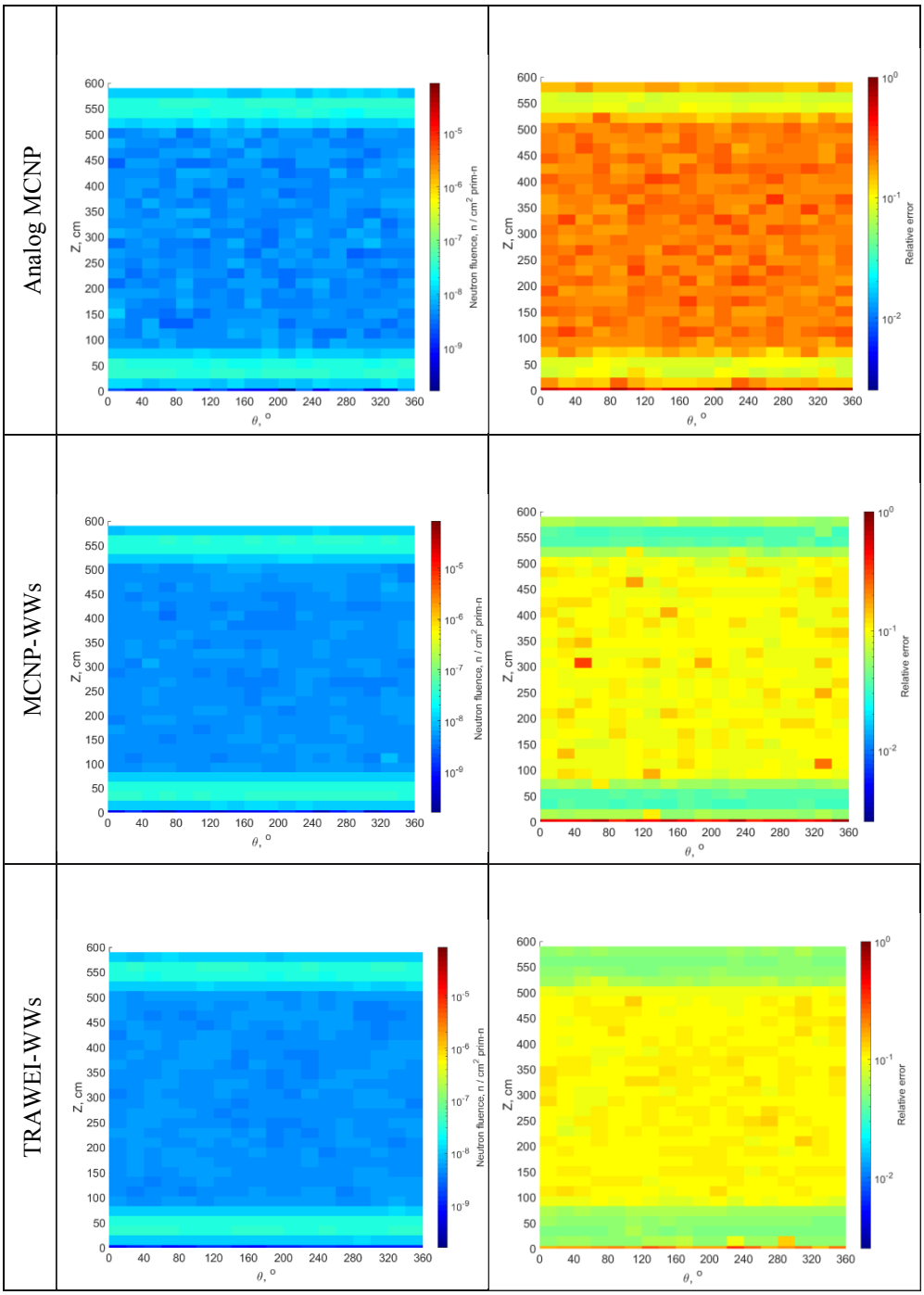

Fig. 3. The left column compares the neutron fluence distribution from different simulations over the surface of cast iron wall; the right column compares the relative error distribution.

TRAWEI (RMC) code is a good option for generating optimal weight values in a single run without requiring multiple iterations or significant computing time. In the future, this developed weight generator tool can significantly contribute to deep penetration shielding calculations and be used for decommissioning studies. The program will be further tested on more real-case problems such as real reactor geometries, and its efficiency will be compared with other weight generation tools such as ADVANTG.

References

1. D. B. Pelowitz, A. J. Fallgren, G. E. Mcmath, *MCNP6 User's Manual, Code version 6.1. 1beta*, Los Alamos, 14-00745 (2014)
2. T. E. Booth, *Sample problem for variance reduction in MCNP*, No. LA-10363-MS. Los Alamos National Laboratory (1985)
3. S. W. Mosher, S. R. Johnson, A. M. Bevill, A. M. Ibrahim, C. R. Daily, T. M. Evans, J. C. Wagner, J. O. Johnson, R. E. Grove, *ADVANTG – an automated variance reduction parameter generator*, ORNL/TM-2013/416 Rev, **1** (2013)
4. J. Sweezy, F. Brown, T. Booth, J. Chiaramonte, B. Preeg, *Automated variance reduction for MCNP using deterministic methods*, Radiation protection dosimetry, **116**(1-4), 508-512 (2005)
5. A. Haghighat, J. C. Wagner, *Monte Carlo variance reduction with deterministic importance functions*, Progress in Nuclear Energy, **42**(1), 25-53 (2003)
6. A. Davis, A. Turner, *Comparison of Global Variance Reduction Techniques for Monte Carlo Radiation Transport Simulations of ITER*, Fusion Eng. Des., **86**, 9–11, 2698 (2011)
7. Q. Pan, K. Wang, *An adaptive variance reduction algorithm based on RMC code for solving deep penetration problems*, Ann. Nucl. Energy, **128**, 171–180 (2019)
8. H. U. Barz, J. Konheiser, *Monte-Carlo Programm TRAMO – Möglichkeiten und Anleitung zur Nutzung*, Report FZR-245, Forschungszentrum Rossendorf, (1998)
9. M. Goldstein, E. Greenspan, *Recursive Monte Carlo Method for Estimating Importance Function Distributions in Deep-Penetration Problems*, Nucl. Sci. Eng., **76**, 308-322 (1980)
10. P. Yadav, R. Rachamin, J. Konheiser, *Weight values for MCNP calculation based on Recursive Monte-Carlo method*, International Conference on Radiation Shielding and 21st Topical Meeting of the Radiation Protection and Shielding Division 521–524 (2022)
11. J. Konheiser, S. Mittag, H. Viehrig, B. Gleisberg, *Application of different nuclides in retrospective dosimetry*, Journal of ASTM International, **9** (2012)
12. F. M. Borst, A. Rimpler, H. Scheib, *Strahlungsmessungen an Transport- und Lagerbehältern zur Beförderung von hochaktiven Glaskokillen aus der Wiederaufarbeitung und von bestrahlten Brennelementen* Report BfS-ET-32/00, Salzgitter (2000)