Computational analysis of the Discrete Ordinates Adjoint Function applicability in VVER Monte Carlo modelling

M Mitev\(^1\), B Ošmera\(^2\), V Smutný\(^3\)

\(^1\)Institute for Nuclear research and Nuclear Energy of the Bulgarian Academy of Sciences, 72 Tsarigradsko shose, 1784 Sofia, Bulgaria
\(^2\)Nuclear Research Institute Řež plc., 250 68 Řež, Czech Republic
\(^3\)Škoda Nuclear Machinery, Orlík 266, 316 06 Plzeň, Czech Republic

mlmitev@inrne.bas.bg

Abstract. The possible use of the adjoint function as an automated source for weight windows generation in the case of VVER-1000 benchmark transport calculations is presented in this paper. The numerical solution for obtaining the adjoint function is performed using the Discrete Ordinates code TORT. Interface software is used to translate the adjoint function into weight windows’ input parameters. A deep penetration problem has been modelled for the VVER-1000 Mock Up, built at the NRI/Rež’s LR-0 critical assembly for VVER-1000 benchmark studies. The neutron flux is evaluated in three locations placed on the azimuthal symmetry axis, radially from the reactor core to the shielding. The calculations are performed in three different approaches: by MCNP code using the weight windows obtained through the adjoint function, by MCNP code using weight windows created by the author through the standard procedure and by the TORT code. The results are compared in terms of integral fluxes and the validity of the adjoint function in variance reduction for VVER reactor Monte Carlo calculations is justified.

1. Introduction

MCNP (Monte Carlo N-Particle) [1] is a general-purpose code that has an extensive application in the nuclear physics research. It is commonly used for modelling detectors response in experiments’ set-ups, cross-sections behaviour, nucleus production from different reactions, etc. This spread is due to the major advantages the Monte Carlo methods have over the other popular method for numerical modelling of particles transport namely Deterministic methods, the most common of which is the discrete ordinates method. Monte Carlo methods are very different from deterministic transport methods. Deterministic methods, solve the transport equation for the average particle behavior. By contrast, Monte Carlo does not solve an equation explicitly, but rather obtains answers by simulating individual particles and recording some aspects (tallies) of their average behavior. The average behavior of particles in the physical system is then inferred (using the central limit theorem) from the average behavior of the simulated particles. Not only are Monte Carlo and deterministic methods very different ways of solving a problem, even what constitutes a solution is different. Deterministic methods typically give fairly complete information (for example, flux) throughout the phase space of the problem. Monte Carlo provides information only about specific tallies requested by the user.

The use of the MCNP code brings number of major advantages from user point of view, namely: possibility to obtain identity of the source and the geometry of the model for calculations with the...
physical object, integrated visualization of the model’s geometry; continuous energy representation of the cross sections available in the software’s libraries.

Important drawback of the Monte Carlo method, connected with its statistical nature, is the necessity of obtaining sufficient statistics for achieving reliable calculational results. This may not be well visible in the aforementioned examples for application, due to the simple geometries and high fluxes typically used in such problems. It is often impossible to reliably evaluate the particle flux using Monte Carlo methods in bigger and more sophisticated systems like nuclear reactors, radiotherapy facility, radioactive waste storage and other such complex facilities within a reasonable amount of time. For this reason less precise numerical approaches, like the Discrete Ordinates method, are still used as a standard in these areas of nuclear physics application.

To reduce the computer time required to obtain results of sufficient precision variance-reducing techniques are used in Monte Carlo calculations in order to decrease the statistical error of the calculations. It is important to note, that the insufficient statistical precision of the calculation is only one of the possible sources of error. For this reason the application of variance reduction techniques does not guarantee a successful calculation and they have to be used appropriately and with caution.

2. The Adjoint Function used in variance reduction technique

The successful use of MCNP’s variance reduction techniques is often difficult, tending to be more art than science. Each variance reduction technique has its own advantages, problems, and peculiarities.

There are four classes of variance reduction techniques introduced in MCNP [1]. Among them the most popular is the Population control class. It is also among those, who bring most value, since app. 50% of the CPU time is spent on tracking of non-important particles [2]. This class of variance reduction techniques controls the particles’ population mainly by splitting them, i.e. increasing their number in regions that are important for the tally, or effectively killing the particles, by using the Russian Roulette principle in regions less important for the tally. Other types of population control techniques are the energy and time cutoff.

The most complex population control technique is the weight window technique [1]. It combines several techniques from its class applying the splitting and rouletting of particles, based on space and energy dependent importance. This technique is one of the most used and effective variance reduction methods that deals with both the direct decrease of variance via a large number of samples (through splitting) and the decrease of simulation time via Russian roulette, and is therefore a very effective variance reduction technique.

Due to its complexity, it is not straightforward to apply Weight Windows in Monte Carlo calculation and significant effort and experience is needed to properly define the necessary input values. Monte Carlo novices, and even more experienced users, are prone to be misled because they do not have enough experience reading and interpreting the summary information on the sampling provided by the MCNP program. Hence, a novice may put more faith in an answer than is justified.

The introduction of automatic weight windows generator in the code has improved things, but the user is still fundamentally responsible for the choice and proper use of the variance reducing techniques. Although the window generator has proved very useful, it is not a panacea for all importance sampling problems, and it is user’s responsibility to decide when the generator's results look reasonable and when they do not. Additionally with the weight window generator it is easy to generate zero weight windows, in a part of the problem’s geometry where either particles do not enter that region or due to particles that did enter the region but did not add to the tally score. The weight window generator calculates the importance of each cell in the problem for the requested response from the calculation. It can be shown, that the adjoint function of the particle flux density brings the same information in specific problems and thus can be used as an automated source for weight windows generation.

The goal of most Monte Carlo particle transport problems is to calculate the response R at some location in the phase space P. This is equivalent to solving the following integral:

\[ R = \int_P \mathcal{P}(P) \sigma(P) dP \]  \hspace{1cm} (1)
where \( \Psi' \) is the particle flux and \( \sigma \) is some objective function in phase space \((r;E,\Omega)\), belonging to \( P \).

It can be shown \cite{3} that the response \( R \) at some location is also given by:
\[
R = \int_{P} \Psi'(P)q(P)dP ,
\]
where \( \Psi' \) and \( q \) are the adjoint function and source density, respectively.

The function \( \Psi' (P) \) has physical meaning as the expected contribution to the response \( R \) from a particle in phase space \( P \), or in other words, the importance of a particle to the response.

After several transformations \cite{3} the following expression for the statistical weight of the particles \( W(P) \) is obtained:
\[
W(P) = \frac{\int_{P} \Psi'(P)q(P)dP}{\Psi'(P)} = \frac{R}{\Psi'(P)}
\]

This equation shows an inverse relationship between the adjoint (importance) function and the statistical weight of the tracked particle in that region of \( P \). Having this determined, one can easily set the boundaries of the weight windows. The adjoint function is being applied as an automated source for weight windows generation used for deep penetration transport calculations in the case of VVER-1000 benchmark \cite{4}.

3. Calculations
Benchmark study was performed to investigate the applicability of the adjoint function as a source for variance reduction in VVER-1000 low statistics Monte Carlo Problem.

3.1. Model description
The LR-0 reactor of NRI/Rez, Czech Republic, has been designed for research of neutron-physical parameters of the VVER type pressurized water reactors. Suitable geometrical conditions and flexible technical arrangements of the LR-0 enable to construct full-scale physical models – Mock-ups of VVER type reactor in radial direction from the core to the biological shielding of the reactor. The simulators of the reactor internals are located inside the LR-0 tank, the pressure vessel and biological shielding simulators - outside the tank but inside the LR-0 shielding room. These full – scale models (Mock-ups) were developed for the research in the dosimetry of VVER pressure vessels and surveillance programs. The VVER-1000 Mock-up is shown on figure 1. Experimental values for two points of the Mock-up have been obtained – behind the RPV model and in the concrete shielding model.

3.2. Calculations
For performing the calculation of the neutron flux, the VVER-1000 LR-0 Mock-up has been modeled in detail in MCNP and TORT \cite{5} codes. The MCNP model with specified points of interest, is shown on figure 2. The model for calculation of neutron flux and the adjoint function by the TORT code is shown on figure 3.
Figure 1. VVER-1000 Mock-up schematic’s horizontal cross section

Figure 2. Horizontal cross section of VVER-1000 Mock-up MCNP model.
3.3. Results
Deep penetration calculations of the neutron flux, that are typical low Monte Carlo statistics problem, have been executed using in three different approaches: (MC) by MCNP code using the weight windows obtained through the adjoint function, calculated by the TORT code, (DO calc) by forward

**Figure 3.** Horizontal cross section of VVER-1000 Mock-up TORT model.

The possible use of the adjoint function as an automated source for weight windows generation in the case of VVER-1000 benchmark transport calculations was investigated. The numerical solution for obtaining the adjoint function is performed using the Discrete Ordinates TORT code. Interface software is used to translate the adjoint function into weight windows’ input parameters (see figure 4).

**Figure 4.** Block-scheme of the method used to generate the input values of the weight windows
solution obtained by the TORT code, using the BGL1000 [6] cross-section data library library, and (DO REF) reference solution by the TORT code, using the BUGLE 96 cross-section data library[7]. Results have been obtained in BUGLE energy structure [7] for the neutron flux with energy above 0.5 MeV. The graphical comparison of these results, normalized per total neutron flux with energy above 0.5 MeV, is shown on figure 5 for Point A (in the concrete shielding of the reactor) and figure 6 for Point B (in the air cavity behind the reactor pressure vessel).

**Figure 5.** Measured and calculated neutron flux with energy above 0.5 MeV for point A

**Figure 6.** Measured and calculated neutron flux with energy above 0.5 MeV for point B
The statistical uncertainty of the MCNP calculation is less than 5%. The results presented on figure 5 and figure 6 show that the three approaches are in good agreement with the experimental values.

4. Conclusion
The successful use of MCNP’s variance reduction techniques is often difficult, tending to be more art than science, and is strongly dependent on the solved problem. The VVER-1000 LR-0 Mock-up was used as a benchmark to investigate the applicability of the adjoint function as source for variance reduction in performing Monte Carlo calculations for VVER-1000 regions with low statistics. The results from the MCNP calculations closely follow the experimental values as well as the reference deterministic calculations, performed with the TORT code. The applicability of the adjoint function and the interface software as an automated source for weight windows generation in the case of VVER-1000 biological shielding is justified.

5. References
[1] Briesmeister J F, MCNP -A General Monte Carlo N-Particle Transport Code, Version4C, LA-13709-M, RSICC ORNL, Code Package, CCC0700, 2000
[2] Saidi P, Sadeghi M and Tenreiro C 2013 IntechOpen, DOI: 10.5772/53384
[3] Wagner J C and Haghighat A 1998 Nucl. Sci. Eng. 128 186
[4] WWER-1000 Mock-up Experiment in the LR-0 Reactor. Mock-up Description and experimental Data. REDOS/R(01)/December 2002/Issue 01, (restricted distribution)
[5] Rhoades W A and Childs R L 1987 TORT Three-Dimensional Discrete Ordinate Neutron/Photon Transport Code, ORNL-6268
[6] Bucholz J A, Antonov S A and Belousov S I 1996 BGL440 and BGL1000 Broad Group Neutron/Photon Cross-Section Libraries Derived from ENDF/B-VI Nuclear Data, IAEA INDC (BUL)-15, Distrib.:G
[7] White J E 1996 BUGLE96, A Revised Multigroup Cross-Section Library for LWR Applications Based on ENDF/B-VI Released 3, ORNL-7795.

Acknowledgments
This work was performed under IAEA project RER0/023 and was supervised by Dr. Bohumil Osmera, LR-0 Unit, Nuclear Research Institute, Rez near Prague.