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Monte Carlo Codes for Neutron Buildup Factors

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ABSTRACT

The point-kernel method is a widely used practical tool for gamma-ray shielding calculations. However, application of that method for neutron transport simulations is very limited. The accuracy of the method strongly depends on the accuracy of buildup factors used in the calculations. Buildup factors are usually obtained using appropriate computer codes, either based on discrete ordinates transport method or Monte Carlo approach. Since these codes put strong demands on computer resources, they are applied on a limited number of shielding configurations and an attempt is made to use these results and formulate an empirical expression for buildup factors estimation. Due to high physical complexity of neutron transport through shielding material it is very hard to perform parameterisation in order to establish adequate empirical formula. Existing formulas are very limited and are usually applicable to a narrow neutron energy range for few commonly used shielding materials, mostly in monolayer configuration.

Recently, a new approach has been proposed for determination of gamma ray buildup factors for mono-layer, as well as multi-layer shielding configurations covering a wide gamma ray energy range. The new regression model is based on support vector machines learning technique, which has theoretical background in statistical learning theory. Development of named regression model required a large number of experimental data obtained by Monte Carlo computer code. More than 7000 Monte Carlo runs were required. Due to physical complexity neutron transport is likely to require even more experimental data in order to generate a model of reasonable accuracy. Therefore, the choice of appropriate Monte Carlo code is a very important question. One has to take into account the accuracy as well as the time required for input preparation and running the code. What also has to be considered is the possibility of the code to be incorporated in an algorithm for automated generation of experimental data.

In this paper three Monte Carlo codes are analysed, namely SCALE4.4 code package (SAS3 sequence), SCALE6.0 code package (MAVRIC sequence), and MCNP5. Two simple experimental setups based on a point isotropic source in spherical and slab-like shield are modelled, and the codes are examined on previously mentioned issues.

The comparison results show that each one of the examined codes has potential to be used for neutron buildup factor model generation. However, some aspects of their utilization require further analysis prior to final selection.

1 INTRODUCTION

The point-kernel method is a widely used practical tool for gamma-ray shielding calculations in shielding design and radiation safety analysis. However, application of that method for neutron transport simulations is very limited. In general, point-kernel method is primarily used for preliminary engineering calculations, where ease and speed are more appreciated than the accuracy obtained by more demanding codes employing transport or Monte Carlo methods, which usually

require more expertise and training to use and are often much slower in reaching the final solution. In the point-kernel approach, the desired quantity (flux, fluence, or dose equivalent) is obtained by multiplying the portion of the quantity resulting from uncollided flux with the parameter called buildup factor, which accounts for the scattered radiation in the medium. It is therefore clear, that the accuracy of the final result is highly dependent on the accuracy of buildup factor used in the calculations.

Buildup factors are usually obtained using appropriate computer codes, either based on discrete ordinates transport method or Monte Carlo approach. Since these codes put strong demands on computer resources, they are applied on a limited number of shielding configurations and an attempt is made to use obtained results and formulate an empirical expression for buildup factors estimation. Due to high physical complexity of neutron transport through shielding material it is very hard to perform parameterisation in order to establish adequate empirical formula. Buildup of scattered neutrons depends strongly on the material composition, incident neutron energy spectrum, and the geometry of the problem [1]. Since the fast neutron scattering cross section is greater than the absorption cross section for most materials, the buildup of scattered neutrons can assume large values. Also the size and shape of the shield medium as well as the energy dependence of the materials cross sections greatly affect the neutron flux density. Therefore, existing neutron buildup factor formulas are very limited and are usually applicable to a very limited neutron energy range for few commonly used shielding materials, mostly in monolayer configuration. For example, Dunn et al. [2] investigated neutron dose-equivalent buildup factors for infinite slabs. Computer experiments were carried out on 6 materials in combination with 7 source neutron energies ranging from 10^{-7} MeV up to 14 MeV, and a simple two-parameter model has been proposed. Values for both parameters differ not only for every material, but also for all energies. Tested 42 material-energy combinations resulted in 42 pairs of different parameters values. Shin et al [3] investigated point isotropic buildup factors for concrete, iron, and a double-layer iron-concrete shield for 7 neutron energies ranging from 400 MeV down to 10 MeV. The proposed empirical formula is based on three parameters for single-layer shield, while the formula for double-layer configurations uses single-layer buildup factors of both materials and a fourth parameter. The parameterisation process resulted in different parameters values for all energies and materials, all together 14 different parameter triples for single-layer shield configurations. The fourth parameter, reguired to calculate double-layer shield configuration, is also energy dependent.

Recently, a new approach has been proposed for determination of gamma ray buildup factors for mono-layer, as well as multi-layer shielding configurations covering a wide gamma ray energy range [4]. The new regression model is based on support vector machines learning technique, which has theoretical background in statistical learning theory [5]. Development of named regression model required a large number of experimental data obtained by Monte Carlo computer code. More than 7000 Monte Carlo runs were required. Since neutron transport, due to high physical complexity, is likely to require even more experimental data in order to generate a model of reasonable accuracy, the choice of appropriate Monte Carlo code is a very important question. One has to take into account the accuracy as well as the time required for input preparation and running the code. What also has to be considered is the possibility of the code to be incorporated in an algorithm for automated generation of experimental data.

Therefore, in this paper three Monte Carlo codes are analysed, namely SCALE4.4 code package (SAS3 sequence), SCALE6.0 code package (MAVRIC sequence), and MCNP5. Two simple experimental setups based on a point isotropic source in spherical and slab-like shield are modelled, and the codes are examined on previously mentioned issues. To validate the accuracy, the results are compared to available references.

Short description of used Monte Carlo codes is given in Section 2. Methodology applied for the analyses of the Monte Carlo codes is presented in Section 3, while the results are given in Section 4. In Section 5 we draw conclusions based on this work. Used references are listed at the end of the manuscript.

2 MONTE CARLO CODES

Based on our previous experience, as well as on available computer codes, we decided to test SCALE code package and MCNP code. Shielding Analyses Sequnce No.3 (SAS3) available in SCALE4.4 [6] code package was used for gamma-ray buildup factors research and proved to be reliable and easy to handle. Therefore, it was also selected for this particular analysis. New version of the SCALE code package, namely SCALE6 [7], does not include SAS3 sequence. Monte Carlo shielding analysis is conducted through MAVRIC sequence. It was therefore reasonable to investigate the applicability of that particular sequence. MCNP code [9] is a widely used tool for neutron transport analyses which triggered our interest in the code and its possibilities in view of neutron buildup factor investigation.

2.1 SCALE code package

The SCALE (Standardized Computer Analyses for Licensing Evaluation) code system was developed at Oak Ridge National Laboratory for the U.S. Nuclear Regulatory Commission to satisfy a need for a standardized method of analysis for the evaluation of nuclear facilities and package designs.

SAS3 sequence is a part of an older version of SCALE code package, namely SCALE4.4 version [6]. It has an automated procedure for coupling cross section processing with Monte Carlo shielding calculations performed by MORSE-SGC, a SCALE version of the MORSE family of Monte Carlo programs. Eight cross-section libraries are automatically available in SCALE4.4 system. We used 27N-18COUPLE library, based on ENDF/B-IV data, which is a 27-neutron-group and 18-gamma-group library widely used and validated in LWR spent fuel shielding calculations. Corresponding neutron energy group structure is given in Table 1.

Table 1 Neutron energy groups of 27N-18COUPLE library (SCALE6)

Group	Upper boundary [eV]	Lower boundary [eV]	Mean [MeV]	Group	Upper boundary [eV]	Lower boundary [eV]	Mean [eV]
1	2.00E+07	6.43E+06	1.32E+07	15	3.05E+00	1.77E+00	2.41E+00
2	6.43E+06	3.00E+06	4.72E+06	16	1.77E+00	1.30E+00	1.54E+00
3	3.00E+06	1.85E+06	2.43E+06	17	1.30E+00	1.13E+00	1.22E+00
4	1.85E+06	1.40E+06	1.63E+06	18	1.13E+00	1.00E+00	1.07E+00
5	1.40E+06	9.00E+05	1.15E+06	19	1.00E+00	8.00E-01	9.00E-01
6	9.00E+05	4.00E+05	6.50E+05	20	8.00E-01	4.00E-01	6.00E-01
7	4.00E+05	1.00E+05	2.50E+05	21	4.00E-01	3.25E-01	3.63E-01
8	1.00E+05	1.70E+04	5.85E+04	22	3.25E-01	2.25E-01	2.75E-01
9	1.70E+04	3.00E+03	1.00E+04	23	2.25E-01	1.00E-01	1.63E-01
10	3.00E+03	5.50E+02	1.78E+03	24	1.00E-01	5.00E-02	7.50E-02
11	5.50E+02	1.00E+02	3.25E+02	25	5.00E-02	3.00E-02	4.00E-02
12	1.00E+02	3.00E+01	6.50E+01	26	3.00E-02	1.00E-02	2.00E-02
13	3.00E+01	1.00E+01	2.00E+01	27	1.00E-02	1.00E-05	5.01E-03
14	1.00E+01	3.05E+00	6.53E+00				

MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) shielding sequence is a part of a new SCALE6 code package [7]. 3-D Monte Carlo calculations are performed through MONACO functional module, which is a MORSE successor. This time, V7-27N19G library has been selected as a cross section library. It has same group structure as 27N-18COUPLE library, but is is based on ENDF/B-VII data [8]. Although fine-group neutron-gamma libraries are available for radiation transport calculations with SCALE shielding modules, we decided to use broad-group library to enable easier comparison of the result.

2.2 MCNP code

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. Pointwise cross-section data are typically used, although group-wise data also are available. For neutrons, all reactions given in a particular cross-section evaluation (such as ENDF/B-VII) are accounted for. We used MCNP5 [9] with pointwise cross-section data based on ENDF/B-VII.

3 METHODOLOGY

The methodological approach is primarily guided by the main goal of this particular research stage, which is to identify the most suitable Monte Carlo code to be used in proceeding analyses of neutron buildup factor determination. To recall, suitability in the context of this research is defined through:

- accuracy of the obtained results compared to reference data,
- time requirements including time needed for input preparation and subsequent input modifications, as well as running time,
- incorporation possibilities implying ease of coupling selected Monte Carlo code with appropriate algorithm for automated neutron buildup factor model generation.

Accuracy and running time are two categories that have to be jointly analyzed. The accuracy of the obtained result represents discrepancy of the result compared to the reference results. But what also has to be taken into account is the Monte Carlo precision, usually expressed as Monte Carlo error on one sigma level defined as one sigma divided by the average value. Running time is closely connected to the desired Monte Carlo error. In practice it means that Monte Carlo description of the specific problem and the number of neutron histories involved in the calculation strongly influence running time, as well as the precision. Depending on problem complexity, a particular Monte Carlo input may or may not lead to satisfactory result, including not only its accuracy but also its Monte Carlo error. In the latter case, modifications on the input are required, usually including changes of parameters controlling variance reduction and the number of analyzed neutron histories. Based on this short elaboration, we decided to predefine desired Monte Carlo error on one sigma level to 5%. Calculation starts with 10,000 histories and an initial set of Monte Carlo parameters controlling variance reduction. In the case that the obtained result breaks 5% error level, the calculation is repeated by increasing the number of neutron histories and modifications of variance reduction parameters. Selection of the initial set of Monte Carlo parameters and number of neutron histories "milestones" is based on our previous experience, as well as on observations made by Dunn et al. [2]

Reference data to which our results are compared to were taken from the research conducted by Dunn et al. [2], Shin et al. [3], and Shirani and Shahriari [10]. That choice also governed experimental setup preparation. Dunn et al. as well as Shirani and Shahriari used point isotropic source in slab-like shields, while Shin et al. used point isotropic source in spherical shields. More attention was put on Dunn et al. as well as Shirani and Shahriari researches, since their investigated energy range is based on neutronics of nuclear power plant operation. On the other hand Shin et al. investigated higher neutron energies corresponding to accelerator facilities. Dunn et al. used a combination of Boltzmann transport equation model for the calculation of uncollided flux and a Monte Carlo model for the calculation of collided flux, while Shirani and Shahriari used Monte Carlo model through MCNP4c code. Shin et al. used S_N code ANISN.

4 RESULTS AND REMARKS

Although three investigated codes have been tested on all variations of two experimental setups and the results have been thoroughly compared to reference material data, in this section only a brief overview of most interesting observations is presented.

4.1 Slab shield experimental setup

In a slab shield experimental setup point isotropic mono-energetic source is placed on one side of the slab shield. Point detector is located on the other side of the shield, opposite to point source. Therefore, the distance between source and detector is equal to the shield thickness. All together, six different materials have been analysed (Table 2). For every material eight different shield thicknesses, expressed by mean free path (mfp) have been modelled (0.5 mfp and 1 mfp up to 7 mfp with the increment of 1 mfp). The mean free path has been calculated as inverse value of the total neutron cross section (1 mfp = $1/\Sigma_t$).

Table 2 Materials analysed in slab shield experimental setup

Material	Density [g/cm^3]	Element	Z	Weight fraction
Aluminium	2.694	Aluminium	13	1.0
Iron	7.86	Iron	26	1.0
Lead	11.33	Lead	82	1.0
Water	1.0	Hydrogen	1	0.1119
		Oxygen	8	0.8881
Polyethylene	0.95	Hydrogen	1	0.1438
		Carbon	6	0.8562
Concrete	2.3	Hydrogen	1	0.00562
		Oxygen	8	0.50010
		Sodium	11	0.01716
		Aluminium	13	0.04577
		Silicon	14	0.31694
		Potassium	19	0.01927
		Calcium	20	0.08290
		Iron	26	0.01224

In this paper, detailed results for water shield with the thickness of 0.5 mfp, 4 mfp, and 7 mfp and lead shield with the thicknesses of 0.5 mfp and 4 mfp, as well as iron shield with the thickness of 4 mfp, are given. Results for water shield are depicted on Figures 1 – 3, and for lead shield on Figure 4 and Figure 5. Graphical representation of buildup factors for 4 mfp thick iron shield is given on Figure 6.

One of the crucial differences between SCALE code package and MCNP5 is the fact that explicit definition of the incident neutron energy is not possible in SCALE, but rather the definition of the "incident" energy group, as given in Table 1. On all figures, SCALE energy group interval is characterized by group mean energy (Table 1).

In the case of water shield, buildup factors obtained by SCALE4.4 (SAS3) are very similar to Shirani and Shahriari [10] on the entire examined neutron energy range. For neutron energies up to 0.01 MeV they are consistently higher than the ones obtained by Dunn et al. [2], with the exception of very thick shield (7 mfp) and low energy of 10^{-7} MeV. For higher energies, behaviour of the results cannot be uniquely characterized, especially for neutron energy of 0.1 MeV. Buildup factors obtained by MCNP5 code are consistently lower than all other buildup factors, except for the lowest energy of 10^{-7} MeV. Similar behaviour was observed for polyethylene and concrete shields.

All SCALE4.4 and MCNP5 results are based on 5% precision premise, and that precision was relatively easy to obtain for thin shields, while for thicker shields number of neutron histories had to be increased up to 1 million. On the average, SCALE4.4 running time can be expressed in seconds, while MCNP5 running time is expressed in tens of seconds.

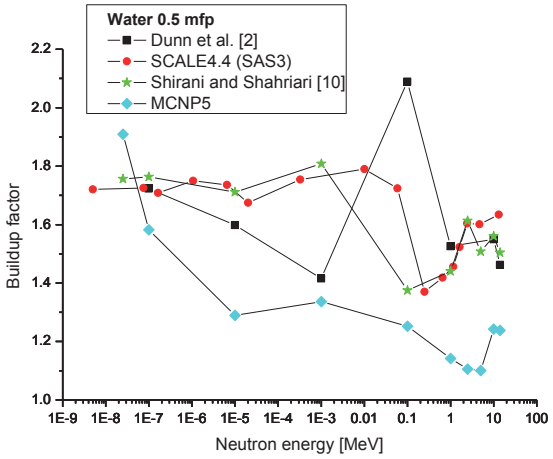

Figure 1: Comparison of buildup factors for 0.5 mfp thick water shield calculated by SCALE4.4 and MCNP5 with reference values extracted from Dunn et al. [2] and Shirani and Shahriari [10]

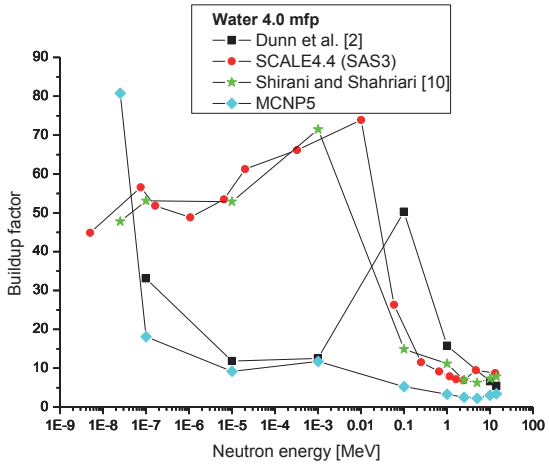

Figure 2: Comparison of buildup factors for 4 mfp thick water shield calculated by SCALE4.4 and MCNP5 with reference values extracted from Dunn et al. [2] and Shirani and Shahriari [10]

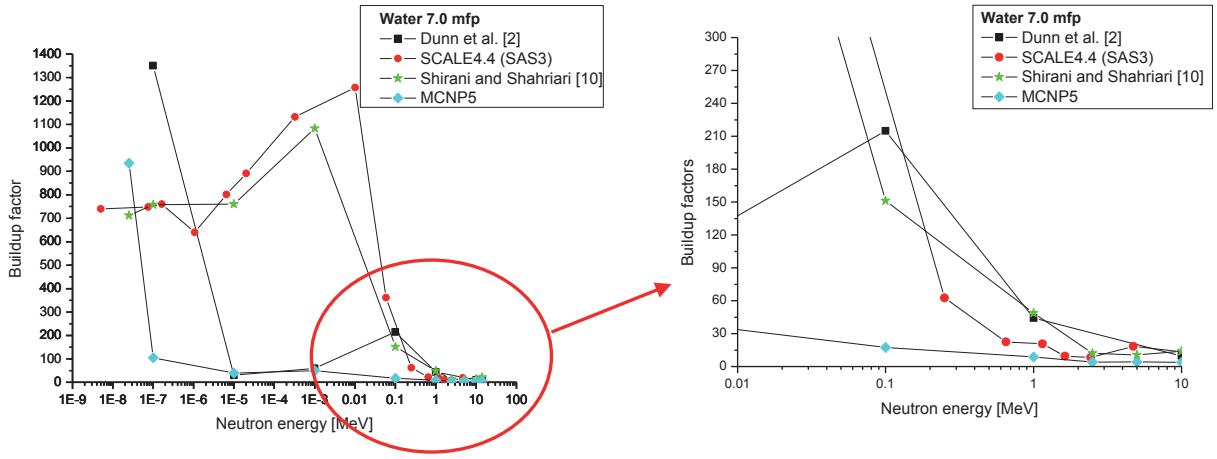

Figure 3: Comparison of buildup factors for 7 mfp thick water shield calculated by SCALE4.4 and MCNP5 with reference values extracted form Dunn et al. [2] and Shirani and Shahriari [10]

In the case of lead shield, buildup factors obtained by SCALE4.4 (SAS3) are very similar to Shirani and Shahriari [10], as well as Dunn et al. [2] for all shield thicknesses and neutron energies up to 1 MeV. For higher energies SCALE4.4 buildup factors have the same behaviour as Shirani and Shahriari, and are higher than Dunn et al. MCNP5 buildup factors are lower than others for neutron energies up to 1 MeV. For higher energies they show stronger dependence on shield thickness, but are generally higher than Dunn et al., and lower than SCALE4.4 and Shirani and Shahriari, except for the neutron energies of 2.5 MeV and 5 MeV. Precise analysis is limited by the fact that Dunn et al. did not analyse these particular energies.

Similar behaviour is observed for iron shields, except for transition towards lower energies. Therefore, the change of behaviour is noticed on neutron energy of 10^{-3} MeV.

4.2 Spherical shield experimental setup

In a spherical shield experimental setup point isotropic mono-energetic source is located in the origin of spherical shield configuration. Shin et al. [3] investigated single-layer (iron and

concrete) and double-layer shield configurations (iron + concrete). Focus of their research was on high neutron energies above 10 MeV. For our research the only interesting energy is 10 MeV. We analysed empirical formula for double-layer shield comprised of iron and concrete obtained by Shin et al. It has to be noted that the formula was developed from data obtained for relatively thick shields were the first (iron) layer is 50+ cm. Our interest was to test the applicability of the formula for thinner shields on neutron energy which represents the energy applicability boundary of the formula. The results for the combinations of 1 mfp of iron followed by 1 mfp, 3 mfp, and 5 mfp of concrete, as well as 3 mfp of iron followed by 1 mfp, 3 mfp, and 5 mfp of concrete are depicted on Figure 7 and Figure 8, respectively.

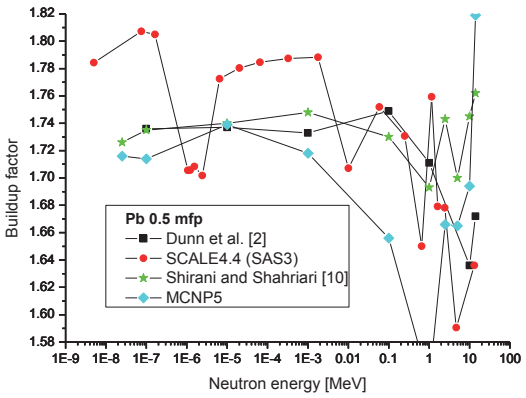

Figure 4: Comparison of buildup factors for 0.5 mfp thick lead shield calculated by SCALE4.4 and MCNP5 with reference values extracted from Dunn et al. [2] and Shirani and Shahriari [10]

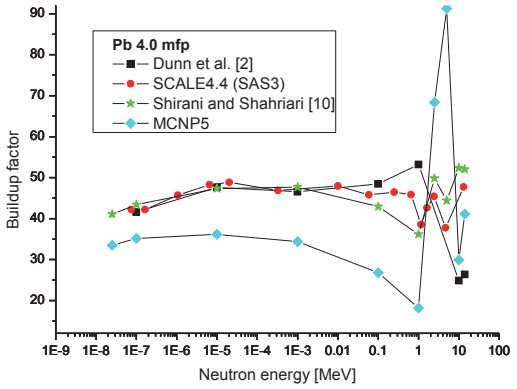

Figure 5: Comparison of buildup factors for 4 mfp thick lead shield calculated by SCALE4.4 and MCNP5 with reference values extracted from Dunn et al. [2] and Shirani and Shahriari [10]

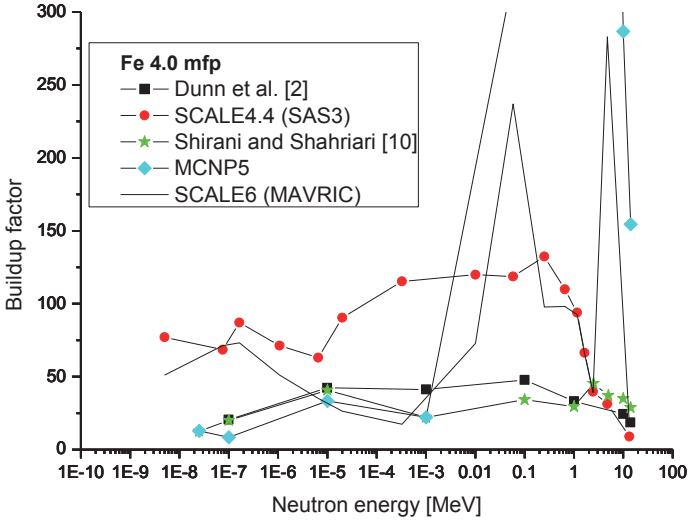

Figure 6: Comparison of buildup factors for 4 mfp thick iron shield calculated by SCALE4.4, SCALE6 and MCNP5 with reference values extracted from Dunn et al. [2] and Shirani and Shahriari [10]

In SCALE, two neutron energy groups (group 1 and group 2 as given in Table 2) were analysed. SCALE4.4, as well as SCALE6 buildup factors are higher than the ones obtained by Shin et al., but they show similar behaviour regardless of first-layer shield thickness (iron). MCNP5 buildup factor behaviour, and the values of buildup factors, show strong dependence on first-layer shield thickness which is obviously connected to MCNP5 treatment of iron in general and has to be analysed in conjunction with results depicted on Figure 6.

The precision of 5% was reached with approximately 1 million neutron histories in all cases. As far as the code's running time, the fastest is SCALE4.4, followed by SCALE6, and finally MCNP5.

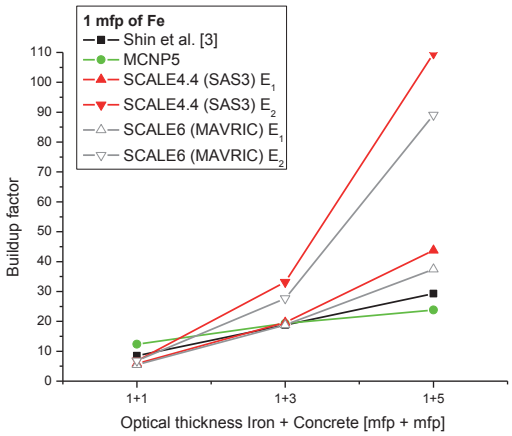

Figure 7: Comparison of buildup factors for double-layer shield comprised of 1 mfp of iron and concrete calculated by SCALE and MCNP5 with reference values extracted from Shin et al. [3]

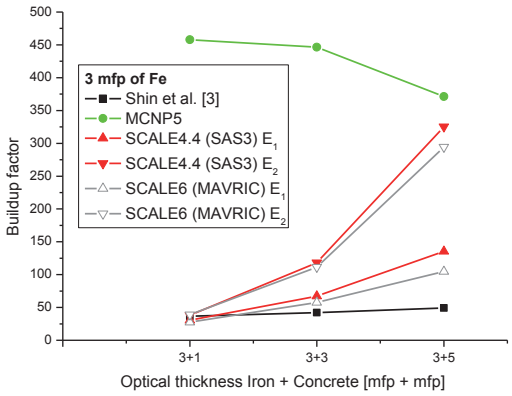

Figure 8: Comparison of buildup factors for double-layer shield comprised of 3 mfp of iron and concrete calculated by SCALE and MCNP5 with reference values extracted from Shin et al. [3]

5 CONCLUSION

In this paper three Monte Carlo codes, namely SCALE4.4 code package (SAS3 sequence), SCALE6.0 code package (MAVRIC sequence), and MCNP5, are analysed for possible application in neutron buildup factor general model development. Two simple experimental setups based on a point isotropic source in spherical and slab-like shield are modelled, and the codes are examined on accuracy, precision, running time, and ease of implementation issues.

Precision of 5% for all three codes can be obtained in reasonable running time measured in seconds or tens of seconds on Quad core 2.66 GHz personal computer. Once the input file is prepared, all three codes can be executed through batch files, and proceeding input file changes can be easily performed. Therefore, the choice of the code by which neutron buildup factor general model is to be developed is primarily based on accuracy and the vision of model applicability.

Although, MCNP5 has the possibility to explicitly define incident neutron energy, which is a desired quality for neutron buildup factor general model development, the behaviour of the code compared to behaviour of SCALE4.4, SCALE6, and reference data is rather unpredictive and requires further analysis.

On the other hand, implementation of SCALE code package for neutron buildup factor model development would imply that the model could be used only for neutron energy groups buildup factor calculations, rather than for particular neutron energy buildup factor calculation.

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