A MCNP SIMULATION STUDY OF NEUTRONIC CALCULATIONS OF SPALLATION TARGETS

by

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The accelerator driven system is an innovative reactor which is being considered as a dedicated high-level waste burner. The function of the spallation target in accelerator driven system is to convert the incident high-energy particle beam to low-energy neutrons. One of the quantities of most interest for practical purposes is the number of neutrons produced per proton in a spallation target. However, this vital value depends not only on the material, but on the size of the target as well, due to the internuclear cascade. The MCNPX 2.4 code can be used for spallation target computation. Some benchmark results have been compared with MCNPX 2.4 simulations to verify the code's potential for calculating various parameters of an accelerator driven system target.

Using the computation method, neutron interaction processes such as loss, capture and (n, xn) into a spallation target have been studied for W, Ta, Pb, Bi, and LBE spallation targets in different target dimensions. With relative errors less than 10%, the numerical simulation provided by the MCNPX code agrees qualitatively with other simulation results previously carried out, qualifying it for spallation calculations. Among the studied targets, W and Ta targets resulted in a higher neutron spallation yield using lesser target dimensions. Pb, Bi, and LBE spallation targets behave similarly regarding the accessible leaked neutron yield on the outer surface of the spallation target. By use of a thicker target, LBE can compete with both W and Ta targets regarding the neutron yield parameter.

Key words: MCNPX code, benchmark, neutron yield, spallation target

INTRODUCTION

Accelerator Driven System. Accelerator driven system (ADS) utilize neutrons produced in a spallation target by a high-energy proton beam to drive a blanket assembly containing both fissionable fuel and radioactive waste. The novel feature of ADS is the presence of a neutron spallation target in the core of the reactor which always operates under subcritical conditions.

The spallation target is ideally conceived as consisting of a high atomic mass material and high-density liquid metals like lead and lead bismuth eutectic (LBE) that fit this requirement extremely well [1].

There is a powerful incentive for improving the precision of code predictions used to simulate the production of neutrons during spallation reactions and the transportation of high and low-energy neutrons within the target material. More realistic codes would ascertain the use of ADS in the future. However, at the moment, there is a need for validating the computational tools and nuclear data for the existing ADS applications.

The MCNPX 2.4 code. The continuous energy of the Monte Carlo code MCNPX 2.4 can be used for modeling neutron transport in critical or subcritical reactors [2].

The MCNPX 2.4 code is a coupling of two previous calculations codes: Los Alamos high-energy transport code (LAHET) [3] and the Monte Carlo N-particle transport code (MCNP) [4]. It allows the treatment of transporting problems in a large range of energies, from a thermal energy of 25 meV to a few GeV.

LAHET generates cross-sections for individual processes, transport nucleons, pions, muons, and antinucleons with an energy $E < 20$ MeV, while the MCNP is able to model the transport of neutrons (and photons and electrons) within the energy range of 10^{-11} MeV $< E <$ 20 MeV. It uses libraries of evaluated data as a source for determining the cross-sections.

The MCNPX simulation of spallation reactions has three stages with a special model used for each of them. The first stage is the intra-nuclear cascade (INC)

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coinciding with the pre-equilibrium stage. This is followed by an equilibrium evaporation that competes with the fission channel (fission fragments undergo an evaporation stage that depends on their excitation energy). After evaporation, a de-excitation of the residual nucleus follows, generating gammas. The MCNPX code enables us to choose different models for the description of individual stages of the spallation reaction. The primary aim of the study presented here is to evaluate, via the comparison between the code output data and experimental works, the uncertainty of the MCNPX code.

Since gaining a better knowledge of neutron economy may have significant consequences regarding the design of high-intensity neutron facilities, the evaluation of the neutron yield of certain heavy targets, while using the MCNPX code, has been in the focus of our work aimed at optimizing spallation targets for ADSR systems.

The spallation process. Spallation is a nuclear reaction in which a relativistic light particle like a proton or a neutron hits a heavy nucleus. The energy of the incoming particle usually varies between a few hundred MeV and a few GeV per nucleon. Spallation is thought to take place in two stages. In the first stage (the intranuclear cascade phase), the incident proton creates a high-energy particle cascade inside the nucleus. During this intranuclear cascade, some high-energy (>20 MeV) secondary particles and low-energy (<20 MeV) cascade particles escape from the nucleus. After the intranuclear cascade, the nucleus is typically left in a highly excited state. In the second stage (the evaporation phase), the excited nucleus relaxes, primarily by emitting low-energy (<20 MeV) evaporation neutrons [5].

In many existing codes, the intranuclear cascade (INC) model is used as a basis for first stage calculations. The description of the nucleon – nucleus reaction in terms of binary nucleon – nucleon collisions inside the nucleus is the basic assumption of the model. In principle, the approach of single INC particles is justified as long as the de Broglie wavelength λ of the cascade particles is smaller than the average intranuclear distance in the nucleus itself (1.3 fm).

Intranuclear cascade calculations follow the history of individual nucleons involved in nucleon – nucleon collisions in a semiclassical manner. In other words, the momenta and coordinates (trajectories) of these particles are treated in a classic manner. The only quantum mechanical concept incorporated into the model is the Pauli principle. The first code of the INC has been created by Bertini [6] in 1963. Later on, Bertini's concept was used in other codes, as well, *e. g* by Yariv in his ISABEL code [7].

The main features of the standard INC approach may be listed as follows: the initial positions of target nucleons are chosen randomly, in a sphere of a radius $R = 1.12\,A^{1/3}$ fm, where A is the mass number of the target nucleus.

The momenta of the nucleons are generated inside a Fermi sphere of P_F = 270 MeV/c. Neutrons and protons are distinguished according to their isospin. All nucleons are positioned in a fixed and constant, attractive potential well of a V_0 = 40 MeV depth, inside the nuclear target volume. The depth value is taken as being a bit higher than the Fermi energy (EF 38 MeV) so that the target remains stable during the reaction [6].

MATERIAL AND METHOD

The spallation target is one of the most important components of ADS. Since a large amount of neutrons is produced by the spallation reaction, one of the essential conditions for selecting the target material is the neutron production rate.

In this study, the MCNPX code system packages have been used to report an uncertainty study on the neutron yield using the Bertini model for a lead target irradiated by 800 MeV protons.

A lead target (diameter 20 cm, height 60 cm) has been simulated by some researchers as a benchmark study using other particle transport codes, such as HETC, SHIELD and so on (tab. 1).

To compare the MCNPX simulation data with other simulation data obtained by different authors, the neutron yield per incident proton of 800 MeV has been calculated for the Pb target. It was evaluated in two energy divisions (<20 MeV and >20 MeV).

This benchmark study has been proposed to determine the neutron yield, number of leaked neutrons of the target surface, leaked neutron spectra, axial dis-

Table 1. Benchmark study of a lead target using different codes [8, 9]

Research group	The used code
ANSALDO (Genoa)	Moving source model + MCNP
JINR (Dubna)	SITHA = Linear transport eq.+ ENDL82
CDF (Paris)	GEANT + FLUKA + GHEISHA
INFN (Milano)	FLUKA + PEANUT
INR (Moscow)	SHIELD = INC + DEECitation + BNAB
ENEA (Roma)	HETC(NEA) + MCNP
IAERI (Japan)	MNTC(JAERI) + MCNP
LANL (Los-Alamos)	LAHET + MCNP
KFA (Julich)	HERMES = HETC(KFA) + MORSE
KfK-1 (Karlsruhe)	HERMES = HETC(KFA) + MORSE
KfK-2 (Karlsruhe)	HERMES = HETC(KFA) + MCNP
KfK-3 (Karlsruhe)	HERMES = HETC(KFA) + MCNP
PSI-1 (Villigen)	HETC(PSI) + TWODANT
PSI-2 (Villigen)	HETC(PSI) + 05R

tribution of the leaked neutrons and, finally, the yield distribution of spallation products into the target according to their mass number; for the final analysis, Bertini, ISABEL, and CEM models have been used. The comparison between the computational data obtained in this work and computational benchmark problems previously outlined by other authors have shown a relative discrepancy.

Regarding target parameters, their material and size determine neutron multiplicity. In principle, the heavier the target nucleus is, the larger the amount of neutrons being produced. The gain factor between heavy and light targets is around a factor of five [10]; however, the radiotoxicity induced in the spallation target can be significantly reduced when using lighter targets [11].

The choice of the optimum spallation target, neutron production rate, unstable residual nuclei produced, as well as target thermal conductivity and its thermal resistance, are parameters of such importance that they warrant special attention.

So, in the second section of this work, the neutron yield per incident proton of 1000 MeV energy has been calculated for Ta, W, Pb, Bi, and LBE targets and the Bertini model used for the simulations.

According to tab. 2, a length of 200 cm has been selected for all the targets so as to minimize the axial neutron leakage and neutron yield calculated for 5, 10, 20, 30, 40, 50, 70, and 100 cm radii of the cylindrical targets with a height of 200 cm.

RESULTS AND DISCUSSION

Neutron yield and leaked neutron number determination. Whereas the number of neutrons produced inside the spallation target and the number of neutrons leaked from the target surface are important parameters, both have been determined in >20 MeV and <20 MeV regions of an 800 MeV proton beam.

Table 2. Target material characteristics

Mat.	Phase state of the spallation target at 454 °C	Melting point [°C]	Density [gcm^{-3}]	Range of 1400 MeV protons [cm]
^{181}Ta	Solid	3017	16.60	58.39
W	Solid	3420	19.30	50.37
Pb	Liquid	327.5	10.44	95.35
^{209}Bi	Liquid	271	9.83	101.55
LBE	Liquid	123	10.11	98.60

The data obtained by MCNPX modeling has been compared with the benchmark study (tab. 3). According to tab. 3, most of the benchmark studies showed the leaked neutron numbers being underestimated in comparison to the ones produced in the target for proton energies of >20 MeV and <20 MeV.

Protons have a parallel angular distribution inside the beam. Additionally, the initial direction of the proton beam is parallel to the axis of the target cylinder and has a uniform spatial distribution over the circular base of the target cylinder.

The statistical uncertainty associated with the Monte Carlo transport simulation results presented in this paper, is less than 4%.

As seen in fig. 1, MCNPX calculations for the total neutron yield have an acceptable agreement with the benchmark data in most of the cases, with an average discrepancy of 8.63%; MCNPX overestimates benchmark data, with the exception of the 2, 6, and 7 group data.

Table 3. Comparison of the benchmark study and MCNPX calculations for neutron production and leakage in the lead target; (target dimensions: radius = 20 cm, height = 60 cm) [9]

Research group	Number of produced neutrons in the target			Number of leaked neutrons of the target surface		
	E_n > 20 MeV	E_n < 20 MeV	Total	E_n > 20 MeV	E_n < 20 MeV	Total
ANSALDO (Genoa)	0.21	10.32	10.53	–	–	–
JINR (Dubna)	0.72	19.47	20.19	0.66	17.33	17.99
CDF (Paris)	1.06	8.43	9.49	–	–	–
INFN (Milano)	–	–	–	–	–	–
INR (Moscow)	2.28	19.46	21.74	0.88	15.43	16.31
ENEA (Roma)	0.95	18.75	19.70	1.3	19.73	21.03
IAERI (Japan)	–	–	–	0.77	19.77	20.54
LANL (Los-Alamos)	2.5	15.79	18.29	1.17	15.02	16.19
KFA (Julich)	1.98	14.59	16.57	0.90	13.37	14.27
KfK-1 (Karlsruhe)	1.98	14.59	16.57	0.80	13.06	13.95
KfK-2 (Karlsruhe)	1.98	14.94	16.92	–	–	–
KfK-3 (Karlsruhe)	1.98	14.69	16.67	–	–	–
PSI-1 (Villigen)	0.11	16.36	16.47	1.5	12.37	13.83
PSI-2 (Villigen)	0.11	16.52	16.63	1.5	14.47	15.97
This work	2.3494	16.375	18.725	1.0748	15.4386	16.5134

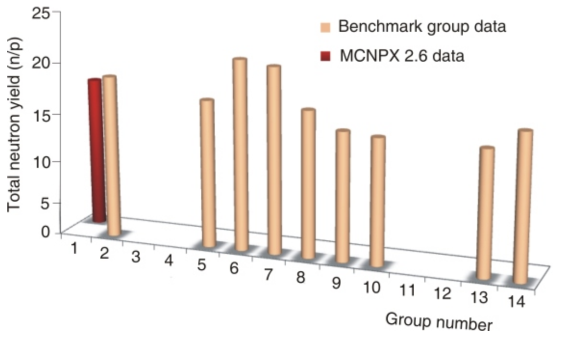

Figure 1. Comparison of total neutron yield achieved some benchmark study and MCNPX code; the lead target dimension: radius = 20 cm, height = 60 cm

Produced and leaked neutron spectra from the target surface

Neutron spectra are the other differential parameter of a spallation target that should be taken into account. As seen in fig. 2, the leaked spectra are softer than the neutron spectra produced in the lead target.

Computational neutron spectra obtained in this work had more agreement with the KFA, LANL, and KfK-1 data.

The axial distribution of the leaked neutrons was determined using MCNPX code calculations. These results were then compared to those obtained otherwise. The axial distribution of the leaked neutrons achieved by the MCNPX code proved to be well-matched with KFA, LANL, and KfK-1 data (fig. 3).

Yield distribution of spallation products. Other important parameters studied in this work are the spallation products predicted by MCNPX. The residual nuclei prediction for the Pb cylindrical target was estimated to be of a 20 cm radius and a 60 cm thickness. The prediction obtained by various intranuclear cascade (INC) models in the MCNPX code, such as the Bertini, ISABEL, and CEN codes, were compared to each other and to the LANL data, as well.

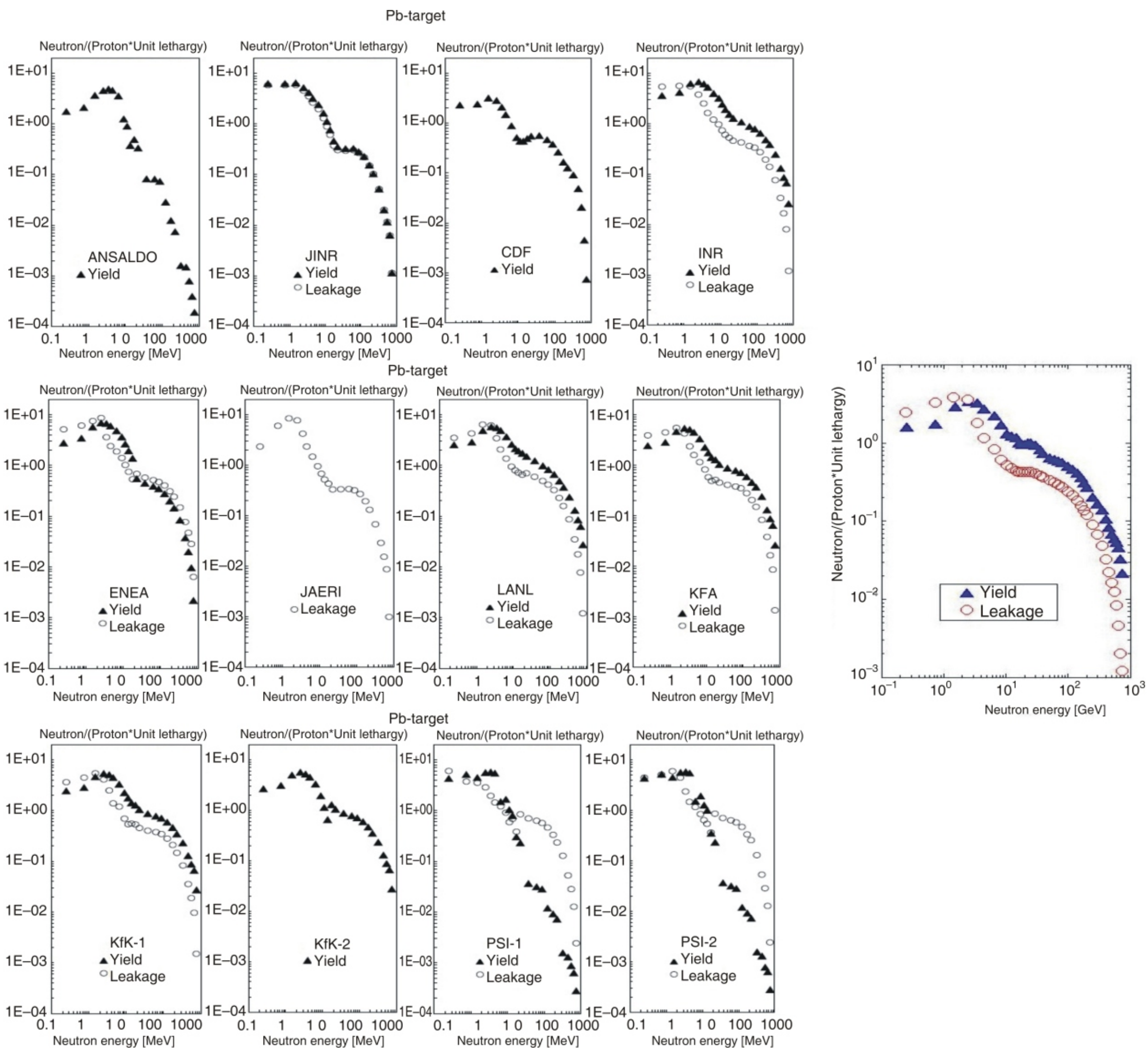

Figure 2. Comparison of neutron spectra achieved some benchmark study and MCNPX code; the lead target dimension: radius = 20 cm, height = 60 cm [9].

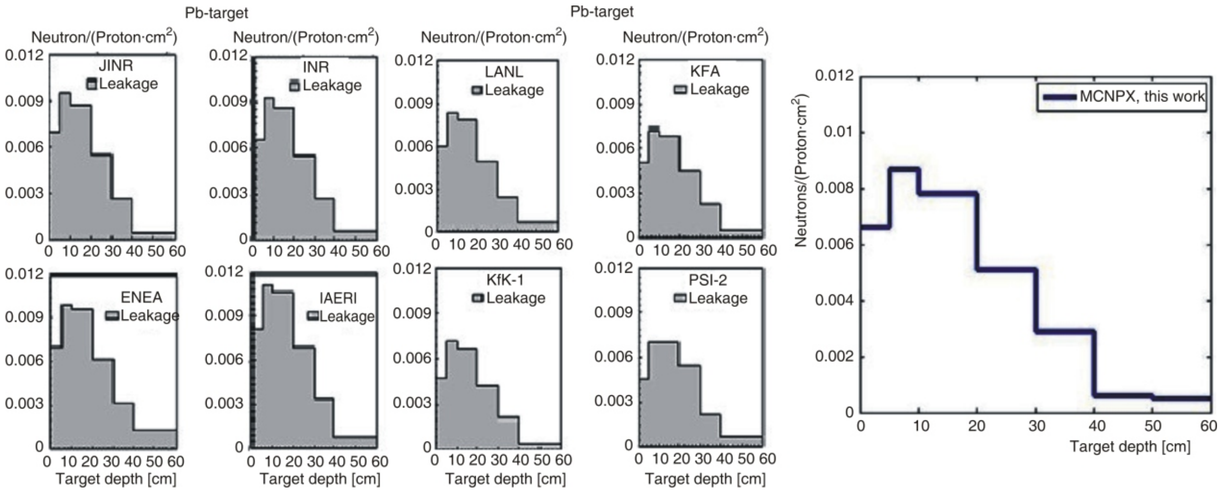

Figure 3. Comparison of axial leaked neutron spectra achieved some benchmark studies and MCNPX code; the lead target dimension: radius = 20 cm, height = 60 cm [9]

The said products spread over two regions of the nuclides chart (fig. 4).

The upper right part corresponds to the heavy, proton-rich residues produced by evaporation (spallation-evaporation products); the central part corresponds to the medium-mass residues produced by fission (spallation-fission products).

As can be seen in the results presented in fig. 4, the data achieved by the Bertini model, overlapped the LANL data more sharply than the others.

According to fig. 4, the yield estimation of spallation products using different models of the intranuclear cascade resulted in more agreements for the Bertini and ISABEL models, with a relative disagreement of less than 5%.

Residual nuclei production using the Bertini model insertion for MCNPX runs has been compared with data obtained by other computation codes (fig. 5).

The results achieved through the use of different codes showed MCNPX code data as well-matched to the LANL and KFA data for estimating the residual nuclei yield.

In accordance with fig. 5, PSI and INR obtained data exhibited noticeable disagreements with the MCNPX results, especially for nuclei $40 < A < 180$.

Overall, code calculations overlap most of the benchmark problems in relative discrepancies of less than 10%.

Calculation of the neutron yield of spallation targets using the MCNPX code. The dimensions of the target play an important role in neutron yield because of the fact that the enhancement of the target radius increases the production of secondary particles involved in another spallation or (n, nx) reaction.

An increase in the radius results in a decrease in the neutron yield via the absorption process. Thus, an optimized radius should be suggested for the spallation target.

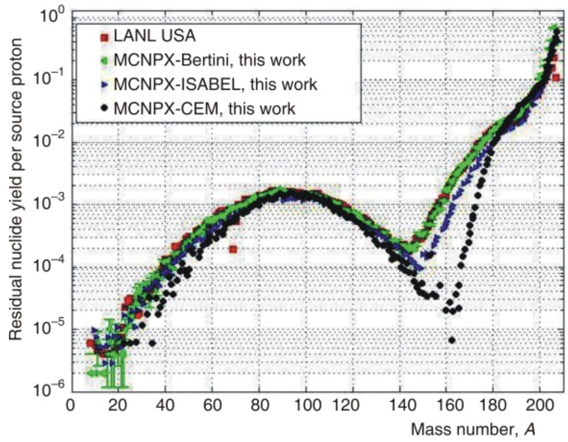

Figure 4. Residual nuclei production in a Pb target by a 0.8 GeV proton beam; the lead target dimension: radius = 20 cm, height = 60 cm

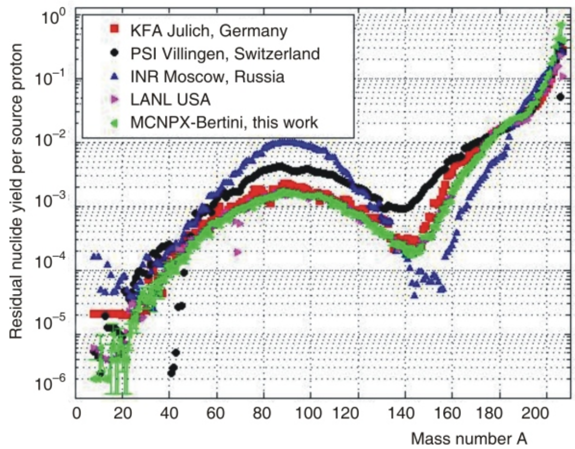

Figure 5. Comparison of residual nuclei production in a Pb target by a 0.8 GeV proton beam using MCNPX code and benchmark studies using other codes; the lead target dimension: radius = 20 cm, height = 60 cm

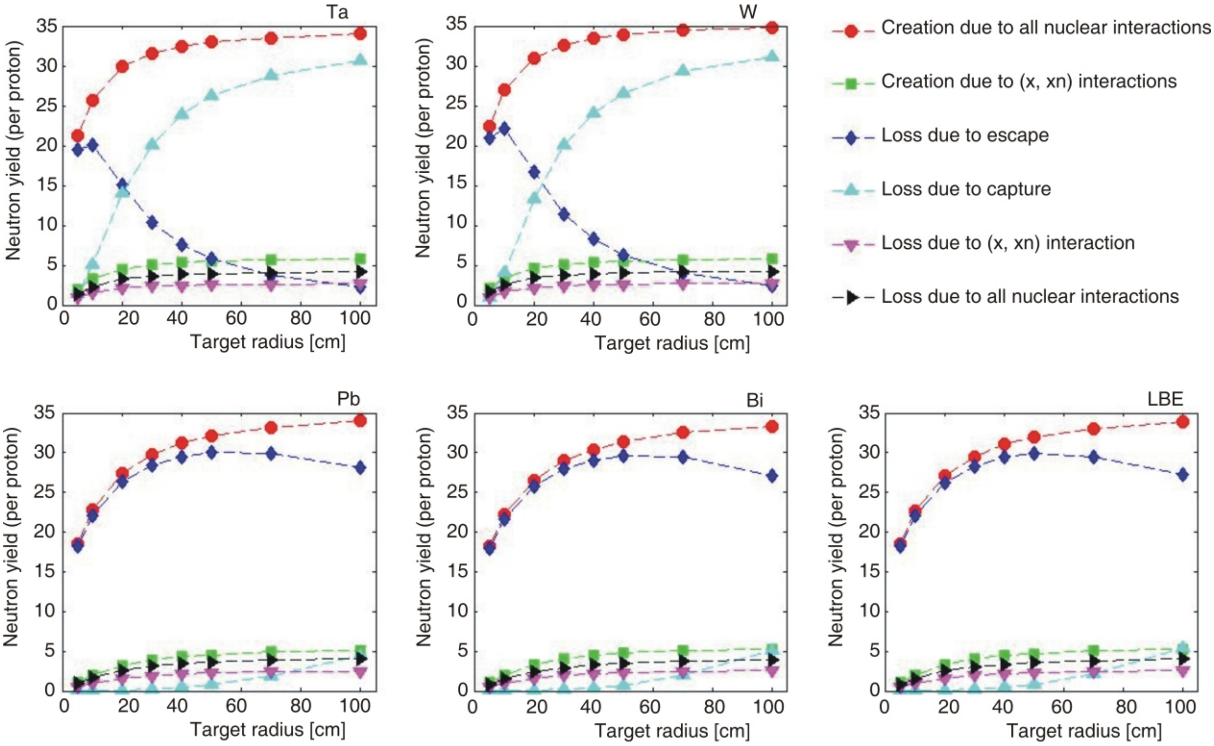

Figure 6. Comparison of neutron interactions in a Pb, Bi, W, Ta, and LBE targets by a 1 GeV proton beam using MCNPX code; height: 200 cm

Different spallation neutron parameters, such as the escaped neutron yield (n, nx) and neutron absorption yield into the spallation target, have been studied for different spallation targets of a 200 cm height and different radii (5, 10, 20, 30, 40, 50, 70, and 100 cm).

Where the atomic number and density of tantalum and tungsten are close to each other during a spallation process, an approximately similar behavior can be predicted. It also seems that lead, bismuth, and lead-bismuth alloys exhibit similarities in prospective neutron yield values. MCNPX outputs for calculating the parameter showed W and Ta accomplishing more total neutron yields than Pb, Bi, and LBE of identical dimensions. However, W and Ta produce less neutron leakage than Pb, Bi, and LBE of identical dimensions. On the other hand, leaked neutrons from a W or Ta surface are noticeably poor because of their high neutron absorption cross-sections (fig. 6).

Tungsten has a higher mass density so that its neutron yield overestimates LBE in identical radii of the targets. In case of a tungsten target, maximum leaked neutrons are obtainable up to a 10 cm radius and more thickness will not exceed the leaked neutron yield noticeably. In contrast, the LBE neutron yield undergoes an obvious enhancement, even up the 50 cm target radius (fig. 7).

Figure 7 clearly indicates that the W target has a markedly higher neutron loss due to the capture process than the LBE in identical radii.

However, the high density and mass number of tungsten can be concluded in a higher neutron yield as a result of more spallations and (n, nx) reactions occurring inside the target.

Liquid targets are more preferable since they are more flexible and withstand mechanical and thermal shocks better.

As for thick targets, high-energy particles escaping from the nucleus over the course of an INC can induce further spallation reactions and generate intranuclear cascades. This pertains chiefly to neutrons, because they do not lose their energy through ionization losses. Thus, among all emitted particles, neutrons penetrate into the target material to the greatest degree. For some target materials, low-energy spallation neutrons (*i. e*., low-energy cascade plus evaporation neutrons) can enlarge neutron production by (n, xn)-reactions. Target materials with a higher density, such as W and Ta, can thus provide a higher efficiency of (n, xn) (fig. 8).

A producible net neutron yield depends not only on the target's mass density, but is also affected by the neutron loss into the target through the capture process. Pb, Bi, and their alloy, LBE, have poorer neutron capture cross-sections than W and Ta. Therefore, target dimension can be expanded without noticeably decreasing the number of neutrons via the capture process (fig. 9).

As has been mentioned, of the three studied targets, Ta and W provide the highest neutron yield into the spallation target. The neutron yield produced in a W target grew by 6% for a thickness between 40-50 cm, while above 50 cm, the neutron yield curve behav-

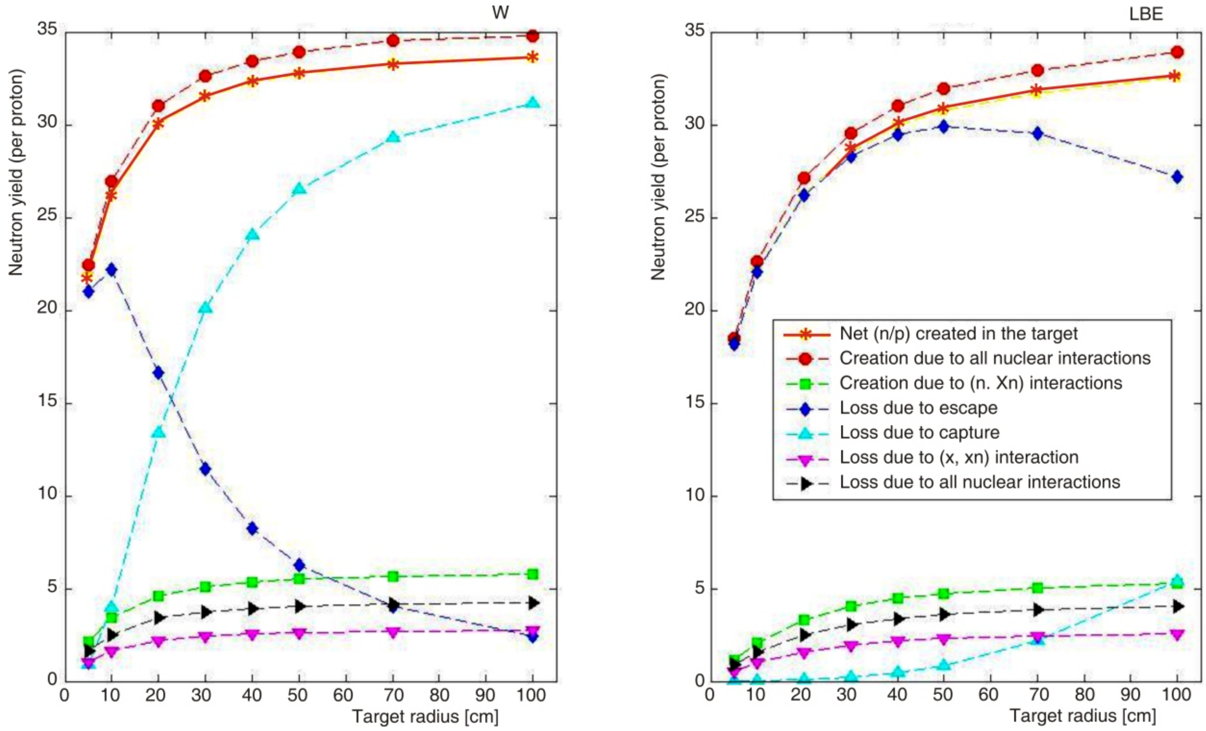

Figure 7. Comparison of neutron yield in W and LBE targets by a 1 GeV proton beam using MCNPX code; height: 200 cm

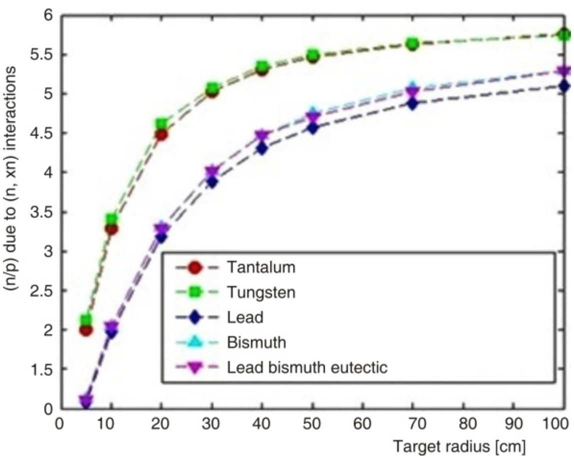

Figure 8. Comparison of neutron number produced via (n, nx) in W , Ta, Pb, Bi, and LBE targets by a 1 GeV proton beam using MCNPX code; height: 200 cm

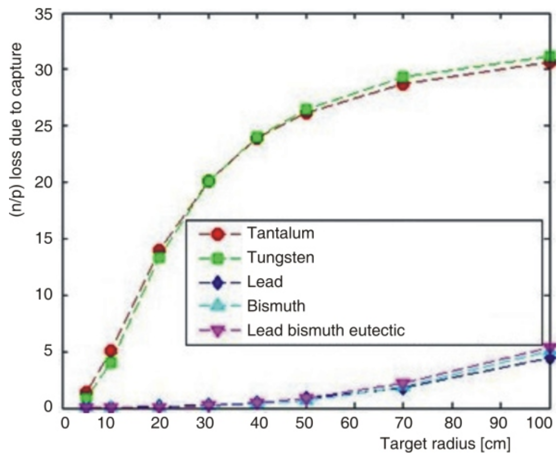

Figure 9. Comparison of neutron loss number via capture in W, Ta, Pb, Bi, and LBE targets by a 1 GeV proton beam using MCNPX code; height: 200 cm

ior seems to be linear. Clearly, after achieving maximum thickness, the neutron yield will decrease as a result of the inability of low energy neutrons to keep up the spallation process or contribute to (n, nx) reactions. The neutron yield produced in a Ta target rose for 3% within the 40-50 cm thickness range. This means that the linear behavior of the curve is activated above the thickness of 40 cm. Pb, Bi, and LBE exhibited highly similar behavior in relation to various degrees of thickness; even up to a thickness of 100 cm, their curves did not show any signs of linear behavior. A striking result of the calculation is that a LBE 50 cm thick can provide the same neutron yield as the one produced in a 20 cm thick W target.

A 100 cm thickness of all compared targets has resulted in approximately identical neutron yields, the maximum discrepancy amounting to 6.5% (fig. 10).

Overall, Ta and W create the highest neutron yield into the target. But, their high neutron absorption cross-sections allow maximum leakage within a 10 cm thickness, with a 22.5 n/p. Despite their lower neutron yields, within the 50 cm range, Pb, Bi, and LBE produce the maximum leaked neutron yield of 30 n/p.

LBE exhibits characteristics similar to Pb and Bi. Hence, its low melting point, 123.5 °C, makes it a choice of interest in view of liquid target handling in ADSR systems.

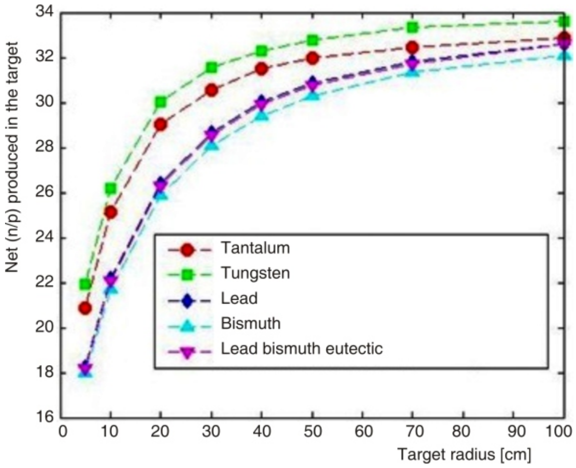

Figure 10. Comparison of neutron yield in W , Ta, Pb, Bi, and LBE targets by a 1 GeV proton beam using MCNPX code; height: 200 cm

CONCLUSIONS

As a powerful computational tool, MNCP 2.4 can provide precise estimations for the determination of the best dimensions for different spallation targets which can result in maximum contained neutron yields.

The neutron yield obtained by the MCNPX code for lead targets showed that the data have an acceptable agreement with the benchmark data obtained by authors using different computational codes, the average discrepancy amounting to 8.63% in most cases.

Among different benchmark studies carried out on neutron spectra emerging from a lead spallation target, KFA, LANL, and KfK-1 data had more agreement with the neutron spectra obtained in the present work. Results show that the MCNPX code is well-matched with LANL and KFA data in estimating the residual nuclei yield. Overall, the code calculations overlap benchmark problems in relative discrepancies of less 10%.

Simulation data show that W and Ta exhibit similar neutronic behavior and that, although they produce the highest neutron yield, because of their high neutron cross-sections, their escaped neutron yield noticeably decreases in radii higher than 10 cm.

The study presented here has shown that Pb, Bi, and LBE exhibit similar neutronic behavior and that, up to a 50 cm radius, there is not much relative discrepancy between the total and the escaped neutron yield.

Regarding the complexities of an ADS target, LBE is suggested because of its low absorption cross-section and highly accessible neutron leakage from the target surface.

AUTHOR CONTRIBUTIONS

Monte Carlo simultions and theoretical analysis were carried out by S. A. H. Feghhi. The manuscript, including figures and tables were prepared and written by S. A. H. Feghhi and Z. Gholamzadeh.

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Сејед АМИР ХОСЕИН ФЕЏИ, Зорех ГОЛАМЗАДЕХ

MCNP СИМУЛАЦИЈА НЕУТРОНСКИХ ПРОРАЧУНА МЕТА ЗА СПАЛАЦИЈУ

Систем управљан акцелератором, нови је облик реактора о коме се размишља као наменском сагоревачу радиоактивног отпада високог нивоа. Функција спалационе мете у систему је да конвертује упадни сноп честица високих енергија у нискоенергетске неутроне. Једна од величина која је од највећег интереса за практичну примену је број неутрона произведен по једном протону у спалационој мети. Међутим, услед интернуклеарне каскаде, број неутрона зависи не само од материјала већ и од величине мете. Програмски пакет MCNPX 2.4 коришћен је за прорачун спалационих мета. Резултати неких тест примера упоређени су са MCNPX 2.4 симулацијом како би се потврдила могућност овог програмског пакета за прорачун разних параметара мете.

Рачунарском симулацијом проучавани су процеси интеракције неутрона као што су губитак, захват и (n, xn) интеракције у спалационој мети, за материјале W, Ta, Pb, Bi и оловно-бизмутну еутектичку смешу (LBE) и за различите димензије мета. Са релативном грешком мањом од 10%, симулација коју даје програмски пакет MCNPX слаже се са резултатима других симулација које су раније обављене – чиме се квалификује за прорачуне спалације. Мете од W и Ta стварале су већи број неутрона при спалацији, употребом мета мањих димензија. Pb, Bi и LBE мете понашале су се слично у погледу могућег доприноса стварању неутрона на спољашњим површинама мете. Коришћењем дебље мете, LBE се може поредити са метама од W и Ta у погледу приноса неутрона.

Кључне речи: MCNPX програм, тест пример, принос неутрона, мета за спалацију