# QUESTIONS OF THE EFFECTIVE METHODS CHOOSING FOR NEUTRON-PHYSICAL PROCESSES SIMULATION

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One of the possible variants of neutron generator is electron accelerator driven subcritical facility. Analytical method is not appropriate one for designing of this system. Such system is simulated by Monte Carlo methods. The main aim of the presented article is choosing of optimal simulation tools by Monte Carlo methods for solution of the neutron-physical tasks.

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## 1. INTRODUCTION

In present moment, as a result of continuously rising price of hydrocarbon fuel, energetic systems based on alternative energy sources, different from hydrocarbon, become more significant. One of the possible variants of such systems is electron accelerator driven subcritical facility. Such systems become more popular in the world. However analytical methods are not appropriate for designing of these systems. In every specific case results, obtained from different methods may differ significantly from each other, especially if the real 3D object is investigated. But there is well-known alternative approach to solve such problems. The simulation is done by Monte Carlo methods i.e. applying direct modelling of the physical process, taking into account the real task geometry. Many kinds of models and algorithms implemented by different program codes for simulation of various physical processes, such as MCNP, MCNPX, PENELOPE, FLUKA, GEANT and others, are well know at present. The main aim of the presented article is choosing of optimal simulation tools by Monte Carlo methods for solution for solving of the neutronphysical tasks, and also for specifying of the boundary conditions for thermo hydraulics tasks in case simulations of electron accelerator driven subcritical facility with electron energy up to 200 MeV.

## 2. SIMULATION CORRESPONDING TO EXPERIMENTS AND ANALYSIS OF OBTAINED RESULTS

At electron beam accelerators the neutrons generated as results of two processes:

• The radiation double conversion. Electrons  $\longrightarrow$  bremsstrahlung radiation  $\longrightarrow$  neutrons from reaction like  $(\gamma, n); (\gamma, 2n); \dots (\gamma, xn)$  and on high Z nucleuses  $(\gamma, F)$  where F is fission product;

• Direct process. Electrons  $\longrightarrow$  neutrons [1]. Therefore to simulate such process it is necessary to use codes which can simulate these processes and real 3D objects. GEANT and MCNPX were selected for these purposes [4], [7]. To verify MCNPX and GEANT codes we provided some photonuclear neutrons production simulation task. Our problem definition corresponds to the real experiments and to other analytical calculations of neutron yields and neutron energy spectra. Comparison of our simulation with experimental data obtained by W.C. Barber and W.D. Georget, [10] was made. Different samples were irradiated by electron beam with energy range 10-35 MeV in this work. To compare our results with experimental data we used the same target geometry and the same beam characteristic as in our experimental work. All targets for this comparison were 4.5 inches square shape. This shape is identical to the shape used in the experiments. The target thickness was also identical to experiment one. Scheme of the experiment is shown on Fig.1.



# Fig.1. Scheme of the experiment by W.C. Barber and W.D. Georget

Neutron yields obtained by GEANT simulation are in good agreement with experiment data for non fission material such as lead, cooper and tantalum.

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However, in case of fissionable material like Uranium, simulation results are about two times less than experimental results. The mean neutron energies obtained from simulation by MCNPX and GEANT codes are 2.71 and 1.32 MeV respectively.

Also neutron spectra distributions simulated by GEANT differes significantly from spectra simulated by MCNPX and experimental data, as it is shown on Fig.2 and Fig.3 respectively.



Fig.2. Neutron spectra simulation of Tantalum irradiated by 34 MeV electrons



Fig.3. Neutron spectra simulation and experimental data of Uranium irradiated by 45 MeV electrons

Analysis of the obtained results shows that GEANT code can be used for neutron yields simulation for non fissionable materials such as Tungsten, Tantalum and Lead. In other words the sampling algorithm based on total photonuclear cross-section seems to be successful as there is no dramatic deviation from experimental results. However the GEANT collaboration physical model, so-called CHIP model (the Chiral Invariant Phase Space model),that is used as base photonuclear model by GEANT simulation [4], [5], [6] does not take into account ( $\gamma$ ,F) reaction for fissionable material such as Uranium. It results in decreasing of neutron yields level. Also it is possible that samplings of the ( $\gamma$ ,2n),...,( $\gamma$ ,xn) channel

reactions are not correct in this case. This results in significant spectra distribution modification. Therefore it is possible to conclude that GEANT code is partly applicable for photonuclear process simulation for non fission material such lead, tantalum. On the other hand for some special cases the GEANT photonuclear models have to be modified and verified with taking into account special task requirements. Unlike GEANT code, the MCNPX code based on direct database interpolation if corresponding database exist [3], [8]. Moreover, MCNPX code is certificated code for neutron physic calculations. The configuration of target geometry and electron beam characteristics and results are shown on Table 1. The mean disagreement between simulated data and experimental data is less than 13% therefore we have very good agreement between MCNPX simulation and experimental data and with GEANT simulation except from Uranium samples, if we take into account that experimental error was 15% and simulation statistical error was less then 0.4%.

Neutron yield versus electron beam energy for different materials is shown on Fig.4 and 5.



Fig.4. Neutron yields versus beam energy for Uranium target



Fig.5. Neutron yields versus beam energy for Tantalum target

Target	Target	Target	Beam	Yield, n/e	Yield,	Ratio,	Yield,	Ratio,
Mate-	thick-	square	ener-	experi-	n/e MC-	sim./exp.	n/e	sim./exp
rial	ness,	shape,	gy,	ment	NPX		GEANT4	
	cm	in	MeV		simula-		simula-	
					tion		tion	
Cu	5.93	$4.5 \times 4.5$	21	5.90E-04	6.60E-04	0.89	4.89E-04	0.83
Cu	5.93	$4.5 \times 4.5$	28	2.14E-03	1.85E-03	0.87	1.58E-03	0.74
Cu	5.93	$4.5 \times 4.5$	34.3	3.34E-03	3.20E-03	0.96	2.58E-03	0.77
Pb	0.519	$4.5 \times 4.5$	19	7.00E-04	6.90E-04	0.99	8.10E-04	1.16
Pb	0.519	$4.5 \times 4.5$	28	1.66E-03	1.35E-03	0.82	1.75E-03	1.05
Pb	0.519	$4.5 \times 4.5$	34.3	2.10E-03	1.53E-03	0.73	2.19E-03	1.04
Pb	3	$4.5 \times 4.5$	19	2.46E-03	2.20E-03	0.9	2.39E-03	0.97
Pb	3	$4.5 \times 4.5$	28	6.70E-03	5.41E-03	0.81	6.14E-03	0.92
Ta	0.374	$4.5 \times 4.5$	19	5.18E-04	6.02E-04	0.86	6.49E-04	1.25
Ta	0.374	$4.5 \times 4.5$	28	1.38E-03	1.47E-03	0.94	1.48E-03	1.07
Ta	0.374	$4.5 \times 4.5$	34.3	1.80E-03	1.82E-03	0.99	1.80E-03	1
U	0.985	$4.5 \times 4.5$	16	2.60E-03	2.11E-03	0.81	1.20E-03	0.46
U	0.985	$4.5 \times 4.5$	21	5.90E-03	5.23E-03	0.89	3.18E-03	0.54
U	0.985	$4.5 \times 4.5$	27.3	1.05E-02	8.89E-03	0.85	5.61E-03	0.53
U	0.985	$4.5 \times 4.5$	35.3	1.50E-02	1.22E-02	0.81	8.01E-03	0.53

Table 1. Comparison of simulation and experiment

Table 2. Comparison of simulation and experiment

Target	Target	Target	Beam	Yield, n/e	Yield,	Ratio,	Yield,	Ratio,
Mate-	thick-	square	ener-	Swanson	n/e MC-	sim./Sw.	n/e	sim./Sw.
rial	ness,	shape,	gy,		NPX	-	GEANT4	
	cm	in	MeV		simula-		simula-	
					tion		tion	
Ta	8.5	$4.5 \times 4.5$	10	1.70E-05	1.72E-05	0.99	2.60E-05	1.53
Ta	8.5	$4.5 \times 4.5$	25	5.29E-03	4.61E-03	0.87	4.19E-03	0.79
Ta	8.5	$4.5 \times 4.5$	34	9.16E-03	8.68E-03	0.95	7.50E-03	0.82
Ta	8.5	$4.5 \times 4.5$	100	3.27E-02	3.12E-02	0.95	2.69E-02	0.82
Ta	8.5	$4.5 \times 4.5$	150	4.97E-02	4.85E-02	0.98	4.26E-02	0.86
U	8.5	$4.5 \times 4.5$	10	1.70E-04	1.67E-04	0.98	4.30E-05	0.25
U	8.5	$4.5 \times 4.5$	25	1.04E-02	1.11E-02	0.94	6.34E-03	0.61
U	8.5	$4.5 \times 4.5$	34	1.66E-02	1.85E-02	0.9	1.13E-02	0.68
U	8.5	$4.5 \times 4.5$	100	5.53E-02	6.61E-02	0.84	3.99E-02	0.72
U	8.5	$4.5 \times 4.5$	150	8.36E-02	1.00E-01	0.83	5.97E-02	0.71
Pb	10	$4.5 \times 4.5$	10	3.22E-05	3.00E-05	0.93	4.10E-05	1.27
Pb	10	$4.5 \times 4.5$	25	5.73E-03	4.87E-03	0.85	5.25E-03	0.92
Pb	10	$4.5 \times 4.5$	34	9.65E-03	8.53E-03	0.88	9.29E-03	0.96
Pb	10	$4.5 \times 4.5$	100	3.36E-02	3.10E-02	0.92	3.41E-02	1.02
Pb	10	$4.5 \times 4.5$	150	8.36E-02	4.73E-02	0.92	5.14E-02	0.62

The next verification step is to compare our simulation with analytical data based on experimental results obtained by W. Swanson [2]. In Swanson's work it is assumed that the entire electromagnetic cascade is totally absorbed in semi-infinite volumes of the chosen materials, but it is disregarded any effect of these media on the resulting neutron fluences. Therefore during simulation we have to take into account these special conditions. Hence during simulations thicknesses of the chosen material were 12 radiation lengths for Uranium, 8 for Lead and more that 9 radiation lengths for Tantalum. Naturally, it is not semi-infinite volume but farther thicknesses increasing during simulation leads to statistics decreasing and increasing influence of the neutron transport process on the neutron fluences that contradict to the Swanson's work assumption. Therefore, with taking into account that bremstralung energy losses is given by formula  $-\frac{dE}{dX} = \frac{E}{X_0}$  where radiation length is  $X_0$ , our simulation conditions quite good correspond to given data. The configuration of target geometry in this case and electron beam characteristics,

Swanson data and simulation results are shown in Table 2. Neutron yield versus electron beam energy for different materials obtained by simulations and by Swanson data are represented on Fig.6, 7 and 8.



Fig.6. Neutron yield for lead target versus initial electron energies



Fig.7. Neutron yield for Uranium target versus initial electron energies



Fig.8. Neutron yield for lead Tantalum versus initial electron energies

Experimental arrangement for time of flight meth-

ods is shown on Fig.9. The mean disagreement between simulated data and Swanson data is less than 9% for MCNPX simulation and 15% for GEANT simulation, except for the Uranium samples. This indicates good agreement between our simulation and given data, with taking into account that Swanson yields overall uncertainty is less or around 20%. The experimental work of D.B. Gayther and P.D. Gooode [9] was selected to compare the neutron energy distributions.

CONCRETE BLOCKHOUSE



Fig.9. Experimental arrangement by D.B. Gayther and P.D. Gooode

In given article the neutron spectra from 45 MeV electron beam irradiated lead and uranium targets was obtained using the time of flight methods.



Fig.10. Neutron spectra for Uranium target

According this article the mean neutron energy for lead target was  $1.92 \pm 0.1$  MeV and for the Uranium target was  $1.37 \pm 0.09$  MeV. This data were obtained from spectra with taking into account effects of neutron moderating by graphite and borated wax collimators and with taking into account scattering effect from neutron transport system. Comparison of the initial neutron energy distributions with simulated ones is shown on figures. As was written above, the neutron energy distribution results simulated by GEANT code in given energy range require more accurate specification of the model parameters and addition calculation verification. This requirement explains the difference between GEANT neutron spectra simulation and experimental neutron energy distributions. Results simulated by MCNPX for the Lead were 1.91 MeV and for Uranium 1.35 MeV. It perfectly agrees with experimental data (see Fig.10 and 11).

The small misfit of the experimental distribution with simulated by MCNPX data is due to geometry and material effects of the experimental arrangement, (see Fig.9) which possibly leads to shift of the initial spectra in low energy range. Unfortunately, in given article is absent any detail information about collimators, including their geometry and size. Therefore there is no possibility to make identical simulation scheme, including detector systems and collimators.



Fig.11. Neutron spectra for Lead target

# CONCLUSIONS

Results of the given investigation shows that for modeling of the photonuclear process it is possible to apply Monte Carlo methods and respectively to done simulations based on the different codes using these methods. However, it is necessary to note that it is important to use the systems that can take into account the special features of the given problem. For example, in our case for modelling of the target electron beam irradiation in energy range up to 200 MeV it is more correct to use MCNPX code, as in this code it is implemented rather new modelling conception. Namely, if corresponding database for particle which interacts with target material exists, the code doesn't use any physical models and use instead of it the direct interpolation of the corresponding experimental data. Naturally, applying of the given methods slightly decreases simulation time, but it is not of such great significance as earlier. On the other hand, modelling of the high energy process or any kind of physical process without experimental databases requires Monte- Carlo codes based on physical models. In this case more preferable is the GEANT system because it is open source code and the model parameters can be easily changed. Also this tool it

is possible to switch between models depending on the problem, or use these models together. All this procedures are more complicated in given version of MCNPX code. Therefore, with taking into account specifications of solved problem, i.e. for modelling of the neutron source generators or subcritical accelerator driven systems, it is preferable to use certificated Monte Carlo codes like MCNPX based on direct interpolation of experimental database, as in this case the simulation results are very close to experimental ones. If we use systems like GEANT, based on physical models, which was developed by GEANT collaboration (CERN), it requires more accurate model parameters investigation and detailed result verification in each special case. The most perspective way is using such systems together. This approach can be used for wide range of tasks, as MCNPX and GEANT systems supplement each other.

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# ПРОБЛЕМЫ ВЫБОРА ЭФФЕКТИВНЫХ МЕТОДИК ДЛЯ МОДЕЛИРОВАНИЯ НЕЙТРОННО-ФИЗИЧЕСКИХ ПРОЦЕССОВ

## И.М. Прохорец, С.И. Прохорец, Е.В. Рудычев, М.А. Хажмурадов, Д.В. Федорченко

Одним из возможных вариантов генератора нейтронов является подкритическая ядерная сборка, управляемая ускорителем заряженных частиц. Для проектирования систем данного типа применение аналитических расчетов является недостаточным. Моделирование таких систем осуществляется методом Монте-Карло. Целью данной работы является выбор оптимального инструмента моделирования методом Монте-Карло для решения нейтронно-физических задач.

# ПРОБЛЕМИ ВИБОРУ ЕФЕКТИВНИХ МЕТОДИК ДЛЯ МОДЕЛЮВАННЯ НЕЙТРОНО-ФІЗИЧНИХ ПРОЦЕСІВ

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Одним з можливих варіантів генератора нейтронів є підкритична ядерна збірка, що керується прискорювачем заряджених частинок. Для проектування систем даного типу застосування аналітичних розрахунків є недостатнім. Моделювання таких систем здійснюється методом Монте-Карло. Метою даної роботи є вибір оптимального інструменту моделювання методом Монте-Карло для вирішення нейтроно-фізичних задач.