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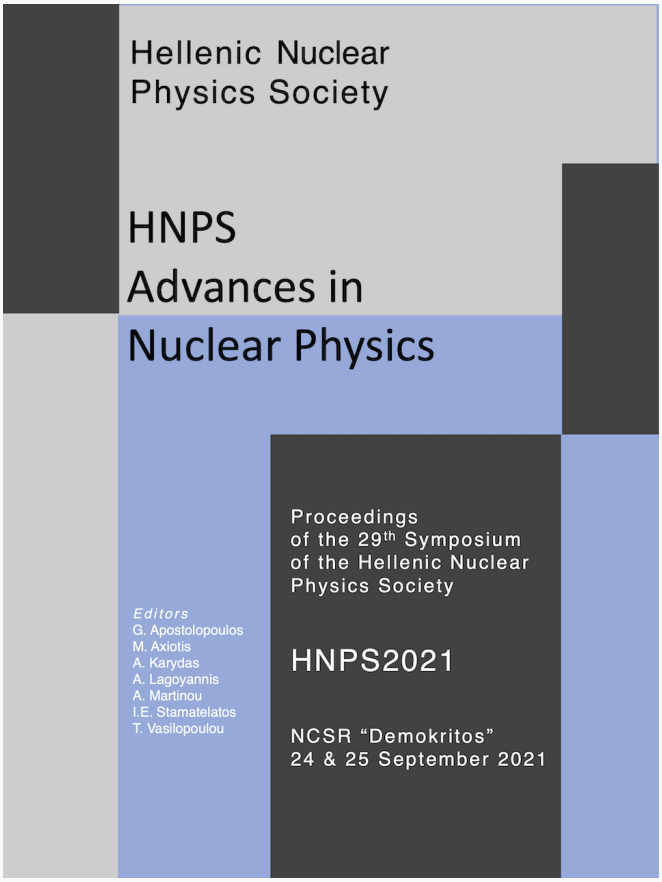

Neutron Dosimetry for In Vitro Biomedical Sample Irradiations

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Neutron Dosimetry for In Vitro Biomedical Sample Irradiations

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Abstract The absorbed dose in vials containing photo-sensitizer solutions irradiated under neutron beams produced by the p-Li, D-D and D-T reactions was calculated. Monte Carlo simulations were performed by coupling the NeuSDesc and MCNP codes in order to derive the neutron energy spectrum, fluence and absorbed dose with depth in the samples. The absorbed dose was estimated taking into account the contributions of all particles (photons, electrons, protons and alpha particles). This study provides important information for the interpretation of in vitro irradiation experiments to be performed under the research program FRINGE aiming to investigate neutron generated electronic excitation as a foundation for a radically new cancer therapy.

Keywords Neutron dosimetry, Monte Carlo simulations

INTRODUCTION

In the framework of the Fluoresence and Reactive oxygen Intermediates by Neutron Generated electronic Excitation as a foundation for radically new cancer therapies (FRINGE) project, a campaign of neutron irradiations will be performed at the Tandem Accelerator Laboratory of the National Centre for Scientific Research “Demokritos” (NCSRD) in Athens (Greece) and at the Swiss Spallation Neutron Source (SINQ) facility at the Paul Scherrer Institut (PSI) in Villigen (Switzerland). Aim of the experiments at NCSRD and PSI is to verify the principles of FRINGE for irradiations with fast and thermal neutron beams, respectively. In this work, the absorbed dose in vials containing photo-sensitizer solutions irradiated with fast neutrons produced by the p-Li, D-D and D-T reactions, as well as for thermal neutrons was calculated. The results of the study provide data necessary for the interpretation of in vitro irradiation experiments to be performed in FRINGE.

MONTE-CARLO SIMULATIONS

Monte-Carlo simulations were performed by coupling the NeuSDesc [1] and MCNP 6.1 codes [2]. Neutron fluence and energy dissipation in the vials was calculated for several different compound and solvent materials. The fast neutron producing reactions used were: ^{7}Li(p,n)^{7}Be, ^{2}H(d,n)^{3}He and ^{3}H(d,n)^{4}He, for neutron energy production at 0.5, 9 and 17 MeV, respectively. For these reactions, the NeuSDesc (Neutron Source Description) code [1] was used to evaluate the expected neutron energy spectra by taking into account the reaction kinematics. The input parameters of the NeuSDesc code are presented in Table 1. For thermal neutrons a beam at 0.025 eV was considered.

The simulation geometry in the MCNP [2] for each neutron producing reaction is presented in Fig. 1, while the cuvette sample, in which the quantities of interest were scored, was divided in 10 slices of 1 mm thickness each. The scoring quantities were the neutron fluence and energy distribution over the cuvette and the energy deposition (+f6) with respect to depth by taking into account all particles in the problem (neutrons, photons, electrons, protons and alpha particles). In addition, several

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compound and solvents (Table 2) were combined in order to evaluate the effect of different solutions on absorbed dose dissipated in the cuvette.

Table 1 *NeuSDesc input parameters for each neutron producing reaction*

Reaction	^{7}Li(p,n)^{7}Be	D(d,n)^{3}He	T(d,n)^{4}He
Target	LiF	Gas	T/Ti
Ion energy (keV)	2240	6135	2448
Gas pressure (kPa)	-	120	-
Gas cell length (mm)	-	37	-
Ti, Li or LiF thickn. (ug/cm2)	55	-	2123.5
T, D/Ti ratio	-	-	1.543
Entrance foil material	-	Molybdenum	Molybdenum
Entrance foil thickness (nm)	-	5000	10000
Directions	90	90	90
Point sources	5	5	5

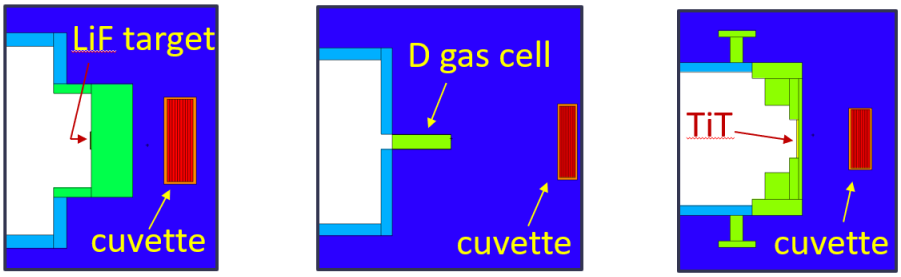

Figure 1 *Representation of the end of the irradiation line along with the flange with the LiF target (left), the deuterium gas cell (middle), the flange with the TiT target (right) and the cuvette which is filled with photosensitizer solution.*

Table 2 Compound and solvent materials that were used in the simulations. The concentration of the final solutions was 10 mM.

Different compounds in DMSO solvent	Different solvents with TPP-Gd-Klaui compound
TPP-Gd-Klaui ($C_{55}H_{51}CoGdN_4O_9P_3$)	DMSO (C_2H_6OS, ρ=1.1004 g/cm^3)
TPP-Gd-Tp ($C_{53}H_{38}BGdN_{10}$)	DMSO-d6 ($(CD_3)_2SO$, ρ=1.19 g/cm^3)
TPFP-Gd-Klaui ($C_{55}H_{31}CoF_{20}GdN_4O_9P_3$)	Acetone (C_3H_6O, ρ=0.7845 g/cm^3)
4OMe-TPP-Gd-Klaui ($C_{59}H_{59}CoGdN_4O_{13}P_3$)	Acetone-d6 ($(CD_3)_2CO$, ρ=0.872 g/cm^3)

RESULTS AND DISCUSSION

The neutron energy distributions as calculated by coupling the NeuSDesc and MCNP codes are presented in Fig. 2. In each spectrum, the main neutron energy peak can be observed at 0.5, 9 and 17 MeV, respectively, along with a low energy neutron tail that can be attributed to scattering. In the case of the 9 MeV simulation (middle subfigure of Fig. 2), an additional peak at ~1.5 MeV exists, which is due to the D(d,pn)D break-up reaction of the deuteron beam on the deuterium gas target. For simulations with thermal neutrons, a monodirectional and monoenergetic neutron disk source was assumed at 0.025 eV, with 2.3 cm radius.

Concerning energy deposition of all particles in the problem (neutrons, photons, electrons, protons and alpha particles) in the cuvette, the results were divided in two categories: in solutions with

the DMSO solvent and different compound materials (Fig. 3) and in solutions with the TPP-Gd-Klaui compound and different solvents (Fig. 4).

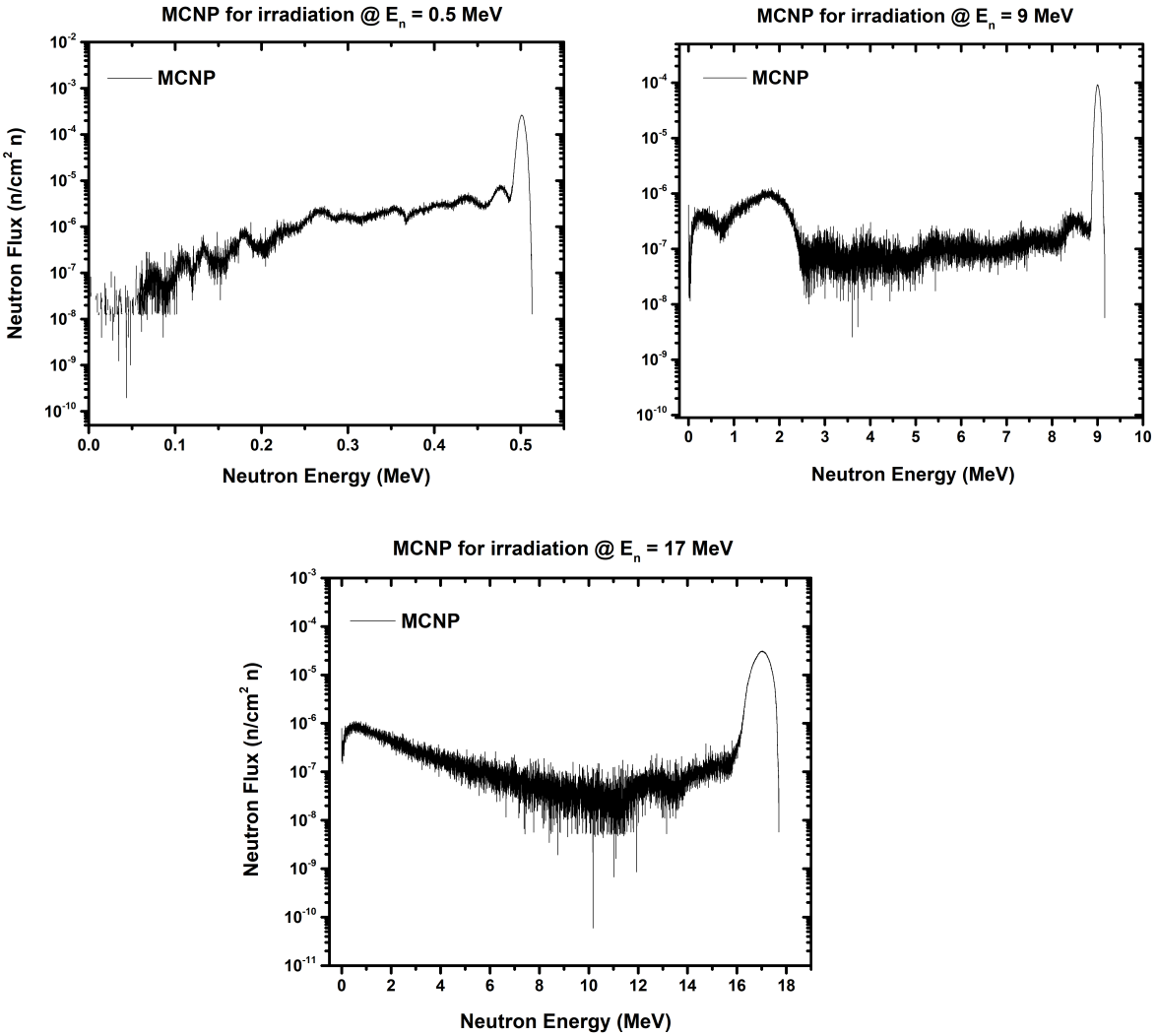

Figure 2 *Neutron energy spectra from the simulations at 0.5, 9 and 17 MeV, as obtained by coupling the NeuSDesc and MCNP 6.1 codes. The statistical errors of the simulations are less than 1%.*

For thermal neutrons (Fig. 3a), the energy deposition is not dependent on the compound, but as expected, it increases of about an order of magnitude when Gd is introduced due to its high thermal neutron capture cross-section. In the case of 0.5 MeV (Fig. 3b), the general trend is a decrease of energy deposition with increasing depth. Similarly, for 9 and 17 MeV (Figs. 3c and 3d), the energy deposition is not dependent on the compound, however a build-up is observed in the energy deposition with respect to the depth in the cuvette at approximately 2 mm and then, the energy deposition is decreasing with depth.

Concerning simulations with different solvents (Fig. 4), when deuterated solvents (DMSO-d6 and Acetone-d6) are used, the energy deposition is approximately an order of magnitude lower than in solutions with hydrogen solvents for neutron energies > 0.5 MeV (Figs. 4b-4d) and this is attributed to the high cross section ratio of neutron scattering over absorption in the deuterated materials, as well as to the dimensions of the irradiated cuvette. The latter means that the scattering process is dominant over absorption for the deuterated samples. In the case of thermal neutrons (Fig. 4a), smaller

differences in energy deposition are observed by using either deuterated or hydrogen solvents and also a build-up occurs at approximately 3 mm depth of the cuvette.

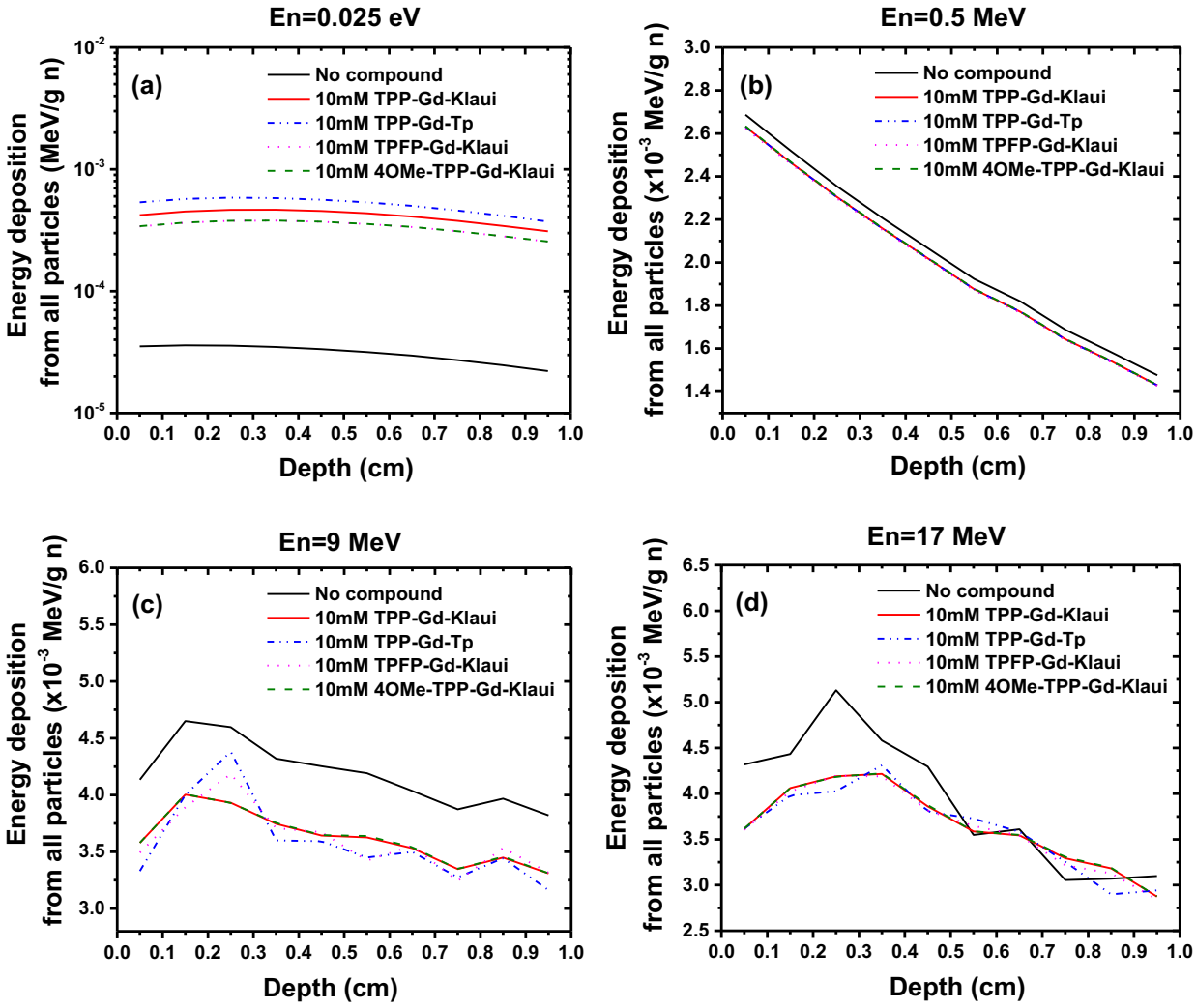

Figure 3 *Energy deposited in the cuvette from all particles in the problem with respect to depth for 0.025 eV, 0.5 MeV, 9 MeV and 17 MeV neutron energies. The statistical errors of the simulations are less than 1%.*

Acknowledgments

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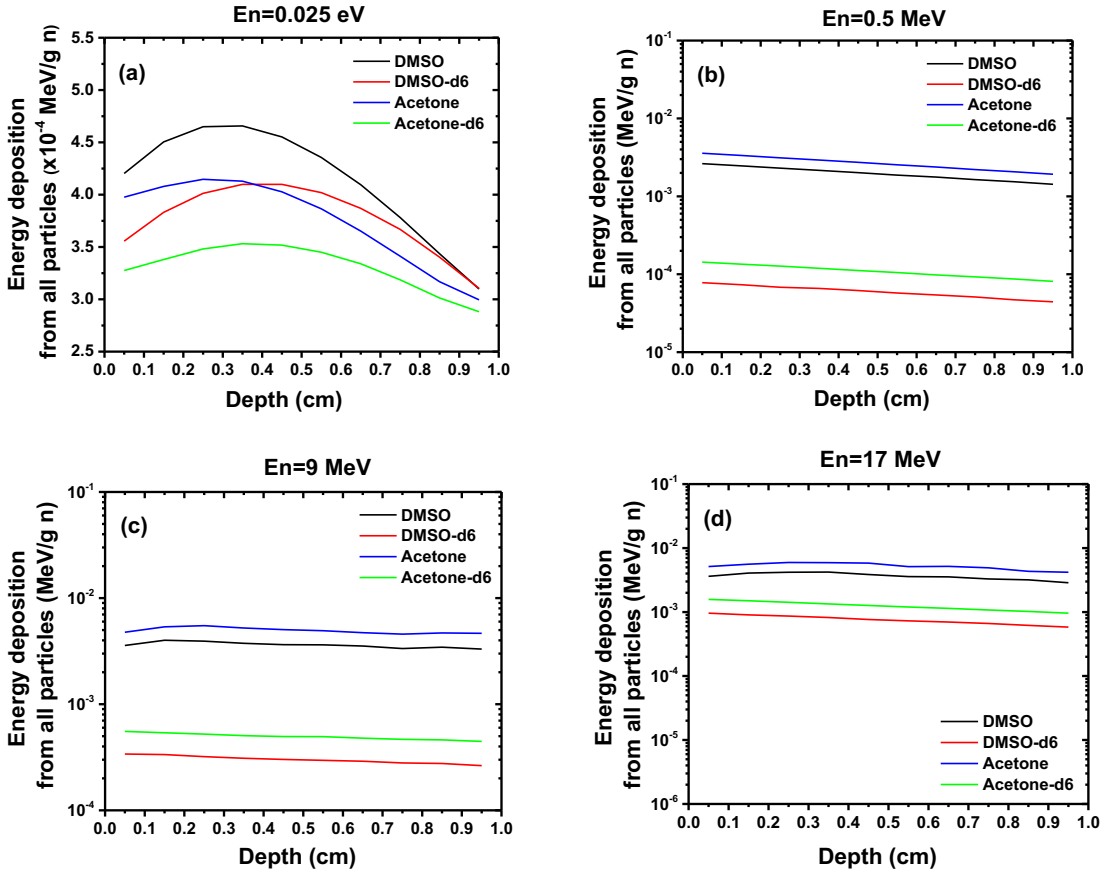

Figure 4 *Energy deposited in the cuvette from all particles in the problem with respect to depth for 0.025 eV, 0.5, 9 and 17 MeV neutron energies, respectively. The statistical errors of the simulations are less than 5%.*

References

[1] E. Birgersson and G. Loevestam, ‘‘NeuSDesc – Neutron Source Description Software Manual’’ 2009. JRC Scientific and Technical Reports.

[2] Initial MCNP6 Release Overview MCNP6 Version 1.0, Los Alamos National Laboratory report LA-UR-13-22934 (2013).