



Investigation of Shielding Parameters of Fast Neutrons for Some Chemotherapy Drugs by Different Calculation Methods

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Abstract:

In this study, we investigated the neutron attenuation properties of twelve different chemotherapy drugs utilizing various computational techniques. The computed fast neutron effective removal cross-section (Σ_R , cm^{-1}) results were compared with empirical formulas, Monte Carlo simulation data obtained from MCNP, MRCsC, and Phy-X/PSD computer program results. Additionally, within each calculation method, the half-value layer (HVL) and the mean free path (λ) values were determined. Our calculations revealed that, when compared to water and paraffin, Gemcitabine, Etoposide, Vincristine, and Doxorubicin exhibited the highest Σ_R values, while Oxaliplatin exhibited the lowest Σ_R value. Understanding and determining the radiation properties of drugs, especially in treatment methods involving radiation, will provide an advantage for both patients and clinical personnel.

1. Introduction

The shielding of fast neutrons holds critical significance in nuclear engineering and radiation protection due to the inherent risks posed by these high-energy particles, generated in nuclear reactions and reactors, to human health and the environment. Effective shielding and the choice of shielding materials are of paramount importance to mitigate these risks. Free neutrons can significantly alter the microstructural properties of a material through elastic or inelastic collisions, nuclear transformations, or ionizations [1,2]. Furthermore, neutrons occurring within biological matter can indirectly cause double-strand breaks in DNA molecules, resulting in cell mutations and fatalities [3]. The effects of neutrons in both living and inanimate materials necessitate a thorough evaluation of radiation shielding. Fast neutrons, typically characterized by energies exceeding 1 MeV, emerge as fundamental components of nuclear reactions. The efficacy of materials in shielding against these neutrons is quantified through the concept of attenuation [4]. Neutron attenuation is calculated using various parameters such as macroscopic effective removal cross-section and

macroscopic thermal neutron cross-section [5,6]. Σ_R is a fundamental quantity used for predicting neutron shielding. Furthermore, it measures potential for energy reduction of fast neutrons through elastic and inelastic collisions within the material [7]. Σ_R is considered as a material property and can be calculated for various protective environments such as alloys [8], ceramics [9], glasses [10], polymers [11], natural minerals [12], as well as rocks, construction, and building materials [13-15]. Neutron shielding materials generally consist of low atomic number elements with high scattering cross-sections that effectively slow down or thermalize incoming neutrons. In practice, small neutron sources are shielded with materials like polyethylene or paraffin, while larger sources necessitate concrete or large water pools/tanks for effective shielding. Cancer treatment often necessitates a combination of modalities, including surgery, chemotherapy, and radiotherapy, depending on the cancer type and stage. One of these treatment methods is chemoradiotherapy, where both chemotherapy and radiotherapy are administered together. After receiving chemotherapy drugs, the patient undergoes radiotherapy and is directly exposed to radiation. Therefore, it is of great importance to investigate the

interaction between these drugs and radiation [16]. In this study, the Σ_R parameters were theoretically calculated for twelve different chemotherapy drugs with varying densities and chemical compositions. The calculated results were compared with empirical formulas, Monte Carlo simulation data obtained from Monte Carlo N-Particle (MCNP, version 5), and results derived from MRCsC and Phy-X/PSD computer programs. Additionally, the half-value layer (HVL) and the mean free path (λ) values were determined for chemotherapy drugs using each of the different calculation methods. This study represents one of the few investigations on Σ_R concerning chemotherapy drugs.

2. Materials and methods

2.1 Theoretical calculation

The total microscopic cross-section of neutrons (σ_t) represents the probability of interaction with the traversed medium. This total microscopic cross-section is the sum of the microscopic scattering cross-section (σ_s) and the absorption cross-section (σ_a). The calculation of the total macroscopic cross-section is expressed in Equation 1.

$$\sigma_t = \sigma_s + \sigma_a \quad (1)$$

A practical method for determining the intensity of neutrons involves obtaining the number of neutrons per unit area or flow rate [17]. The decay of neutrons within a material can be likened to the Lambert-Beer Law, which is commonly used for the absorption of photons. The formula for neutron decay intensity is presented in equation 2 [18,19].

$$I = I_0^{-\Sigma_t x} \quad (2)$$

In this equation, I_0 represents the initial neutron density, while I denotes the neutron density passing through the attenuator thickness (x , cm). Σ_t represents the total macroscopic cross-section. Σ_R is the probability of a fast or fission-energy neutron undergoing its first collision. Empirical approaches are used to obtain mass removal cross-section (Σ_R/ρ , cm²/g) values for certain elements lacking experimental data. Since chemotherapy drugs are composed of multiple elements, calculating Σ_R requires the use of the Σ_R/ρ rule for constituent elements. One of the empirical models is detailed in equations 3 and 4 [20].

$$\Sigma_{R/\rho} = 0.190 Z^{-0.743} Z \leq 8$$

$$\Sigma_{R/\rho} = 0.125 Z^{-0.565} Z > 8 \quad (4)$$

Generally, protective materials are composed of chemical compounds or mixtures. The macroscopic removal cross-sections are computed from the Σ_R values of the constituent elements and are presented equation 5 [5, 21-23].

$$\Sigma_R = \sum_i \rho_i (\Sigma_{R/\rho})_i \quad (5)$$

In this equation, ρ_i , ρ and $(\Sigma_{R/\rho})_i$ represent the partial density of the first component (g/cm³), the density, and the mass removal cross-section, respectively. The formula for partial density is provided in Equation 6.

$$\rho_i = \sum_i w_i \rho_s \quad (6)$$

Here, w_i and ρ_s represent the weight fraction of the i^{th} component (element or compound) and the total density of the material, respectively. The half-value layer (HVL) expresses the thickness of the material that reduces incoming neutron radiation by half. HVL can be calculated for neutrons using equation 7 [24,25].

$$HVL = \frac{\ln 2}{\Sigma_R} \quad (7)$$

The mean free path (λ) is defined as the distance traveled by neutrons within the interaction materials and can be computed using equation 8 [25,26].

$$\lambda = \frac{1}{\Sigma_R} \quad (8)$$

The MRCsC and Phy-X/PSD program

The user-friendly software "MRCsC," comprises a front-end and back-end processor, an analytical model, and an integrated database. It has been meticulously developed as an efficient tool for radiation shielding design. MRCsC is engineered to provide reliable predictions of the macroscopic effective removal cross-section of fast neutrons for various materials [27]. An accessible web-based software tool called Photon Shielding and Dosimetry (PSD) has been developed to simplify the computation of dosimetry and shielding-related parameters. This software is able to generate comprehensive data on shielding parameters covering the continuous energy range in different energy ranges [28].

3. Results and Discussion

The Σ_R values of twelve different chemotherapy drugs have been computed by using the theoretical

Table 1. Chemical properties of chemotherapy drugs

Molecule	Chemical formula	Mol. weight (g/mole)	ρ (g/cm ³)
Cisplatin	PtCl ₂ H ₆ N ₂	300.04	3.74
Methotrexate	C ₂₀ H ₂₂ N ₈ O ₅	454.44	1.50
Oxaliplatin	C ₈ H ₁₄ N ₂ O ₄ Pt	397.29	1.01
Ifosfamide	C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P	261.09	1.35
Gemcitabine	C ₉ H ₁₁ F ₂ N ₃ O ₄	263.20	1.83
Fluorouracil	C ₄ H ₃ FN ₂ O ₂	130.08	1.51
Pemetrexed	C ₂₀ H ₁₉ N ₅ Na ₂ O ₆	471.37	1.02
Etoposide	C ₂₉ H ₃₂ O ₁₃	588.56	1.61
Vincristine	C ₄₆ H ₅₆ N ₄ O ₁₀	824.96	1.43
Tamoxifen	C ₃₂ H ₃₇ NO ₈	563.64	1.00
Paclitaxel	C ₄₇ H ₅₁ NO ₁₄	853.90	1.42
Doxorubicin	C ₂₇ H ₂₉ NO ₁₁	543.51	1.60

Table 2. Elemental composition of twelve different chemotherapy drugs [29]

Molecule	H	C	N	O	Cl	Pt	P	F	Na
Cisplatin	0.0201		0.0933		0.2363	0.6501			
Methotrexate	0.0487	0.5286	0.2465	0.1760					
Oxaliplatin	0.0355	0.2418	0.0705	0.1610		0.4910			
Ifosfamide	0.0579	0.3220	0.1072	0.1225	0.2715		0.118		
Gemcitabine	0.0421	0.4107	0.1596	0.2431				0.1443	
Fluorouracil	0.0232	0.3693	0.2153	0.2459				0.1460	
Pemetrexed	0.0406	0.5096	0.1485	0.2036					0.0975
Etoposide	0.0548	0.5918		0.3533					
Vincristine	0.0684	0.6697	0.0679	0.1939					
Tamoxifen	0.0661	0.6819	0.0248	0.2270					
Paclitaxel	0.0601	0.6610	0.0164	0.2623					
Doxorubicin	0.0537	0.5966	0.0257	0.3237					

Table 3. Comparison of different chemotherapy drugs ΣR from MCNP, MRCsC, Phy-X/PSD and empirical fit

Materials	(ΣR) cm ⁻¹				PD* MRCsC- Phy-X/PSD	PD* MCNP - $\Sigma R/\rho$
	MRCsC	Phy-X/PSD	MCNP	Estimation using $\Sigma R/\rho$ of elements		
Cisplatin	0.1276	0.1090	0.1038	0.1085	14.57	4.52
Methotrexate	0.1204	0.1108	0.0953	0.1055	7.97	10.70
Oxaliplatin	0.0548	0.0480	0.0441	0.0487	12.40	10.43
Ifosfamide	0.1104	0.0955	0.0897	0.0952	13.49	6.13
Gemcitabine	0.1346	0.1244	0.1140	0.1241	7.57	8.85
Fluorouracil	0.0933	0.0865	0.0785	0.0864	7.28	10.06
Pemetrexed	0.0759	0.0698	0.0627	0.0692	8.03	10.36
Etoposide	0.1349	0.1236	0.1105	0.1238	8.37	12.03
Vincristine	0.1343	0.1221	0.1106	0.1227	9.08	10.94
Tamoxifen	0.0925	0.0841	0.0758	0.0842	9.08	11.08
Paclitaxel	0.1257	0.1143	0.1025	0.1142	9.06	11.41
Doxorubicin	0.1334	0.1222	0.1092	0.1224	8.39	12.08
H ₂ O	0.1103	0.1030	0.1000	0.1030	6.61	3.00
Paraffin, C ₂₅ H ₅₂	0.1417	0.1223	0.1190	0.1220	13.69	2.52

*Percentage deviation

respectively. The discrepancies observed in neutron attenuation coefficients among the calculation methods are notable. MCNP consistently yielded lower coefficients compared to MRCsC, estimation and Phy-X/PSD. These variations might be attributed to the inherent assumptions and approximations each method employs. MCNP, for instance, assumes a simplified molecular structure, potentially underestimating neutron interaction probabilities compared to the more intricate representations in MRCsC, estimation and Phy-X/PSD. The molecular composition of the drugs appears to significantly impact their neutron attenuation capabilities. Oxaliplatin, with a higher Z content of, consistently exhibited lower shielding efficiency across all calculation methods. This reinforces the idea that the elemental composition and molecular structure play pivotal roles in neutron attenuation. Table 3 presents the ΣR values of chemotherapy drugs obtained using various calculation methods. In the study conducted by Hila et al. (2023), fast neutron mass removal cross-sections ($\Sigma R/\rho$, cm^2/g) based on ENDF/B-VIII.0 were numerically generated using the sliced spherical shell MCNP Monte Carlo model under different neutron source spectra ($^{241}\text{Am-Be}$, ^{252}Cf , ^{235}U). The values in Table 3 about MCNP were obtained from this study. In this study, the ΣR values were computed using the $\Sigma R/\rho$ values obtained using Californium-252 (^{252}Cf). According to Table 3, in all calculation methods, Paraffine (0.1417 cm^{-1}) has been found to be the closest to chemotherapy drugs, including Gemcitabine (0.1346 cm^{-1}), Etoposide

(0.1349 cm^{-1}), Vincristine (0.1343 cm^{-1}), and Doxorubicin (0.1334 cm^{-1}). With the exception of Tamoxifen (0.0925 cm^{-1}), Pemetrexed (0.0759 cm^{-1}), Fluorouracil (0.0933 cm^{-1}), and Oxaliplatin (0.0548 cm^{-1}), the ΣR values of all other chemotherapy drugs are higher than that of water (0.1103 cm^{-1}). In the study conducted by Aygün and Karabulut (2020), a simulation method was employed to investigate the gamma and neutron interactions of select cancer drugs. Similar to our study, they found that the Oxaliplatin has a lower ΣR value compared to other drugs. This result suggests that an increase in the content of low atomic number (Z) elements within the compound leads to an increase in the ΣR value. Furthermore, the presence of hydrogen within the compound significantly contributes to elevated ΣR values, as the $\Sigma R/\rho$ value for hydrogen is nearly double that of other elements. Consequently, compounds with higher hydrogen content exhibit increased ΣR values, a phenomenon that has been corroborated by Akyıldırım's study on basic carbohydrates (2019), focusing on fast neutron shielding parameters.

Understanding the shielding parameters of chemotherapy drugs against fast neutrons is crucial, especially in radiation therapy settings where unintended exposure can impact treatment outcomes. These findings underscore the importance of considering the molecular makeup of drugs when evaluating their potential shielding effectiveness.

Table 4. Comparison of HVL and λ results with different calculation method

Materials	(HVL) _{MRCsC}	(λ) _{MRCsC}	(HVL) _{Phy-X}	(λ) _{Phy-X}	(HVL) _{MCNP}	(λ) _{MCNP}	(HVL) _{Zoller}	(λ) _{Zoller}
Cisplatin	5.4310	7.8370	6.3577	9.1743	6.6729	9.6287	6.3833	9.2111
Methotrexate	5.7558	8.3056	6.2545	9.0253	7.2684	10.4883	6.5657	9.4743
Oxaliplatin	12.6460	18.2482	14.4375	20.8333	15.7044	22.6614	14.2123	20.5083
Ifosfamide	6.2772	9.0580	7.2565	10.4712	7.7242	11.1461	7.2777	10.5017
Gemcitabine	5.1486	7.4294	5.5707	8.0386	6.0778	8.7703	5.5698	8.0373
Fluorouracil	7.4277	10.7181	8.0116	11.5607	8.8542	12.7766	8.0132	11.5631
Pemetrexed	9.1304	13.1752	9.9284	14.3266	11.0495	15.9444	10.0104	14.4452
Etoposide	5.1371	7.4129	5.6068	8.0906	6.2686	9.0456	5.6048	8.0877
Vincristine	5.1601	7.4460	5.6757	8.1900	6.2655	9.0411	5.6736	8.1870
Tamoxifen	7.4919	10.8108	8.2402	11.8906	9.1417	13.1915	8.2433	11.8951
Paclitaxel	5.5131	7.9554	6.0630	8.7489	6.7566	9.7498	6.0635	8.7497
Doxorubicin	5.1949	7.4963	5.6710	8.1833	6.3446	9.1552	5.6744	8.1881
H ₂ O	6.2828	9.0661	6.7281	9.7087	6.9300	10.0000	6.7281	9.7087
Paraffin	4.8906	7.0571	5.6663	8.1766	5.8235	8.4033	5.6803	8.1967

Moreover, this insight might guide the design and development of new drugs optimized for both therapeutic efficacy and radiation safety. Table 4 presents the computed HVL and λ values using different calculation methods. Lower HVL and λ values indicate better neutron stopping capabilities. Paraffin (4.8906 cm) has the closest HVL values to Gemcitabine (5.1486 cm), Etoposide (5.1371 cm), Vincristine (5.1601 cm), and Doxorubicin (5.1949 cm). The highest λ values were obtained using MCNP method. According to this, the highest λ values are found for Tamoxifen (13.1915 cm), Pemetrexed (15.9444 cm), Fluorouracil (12.7766 cm), and Oxaliplatin (22.6614 cm). Greater λ values signify deeper penetration of fast neutrons for drugs with high λ values compared to those with low λ values. The variations in results across different calculation programs can be attributed to discrepancies in their data libraries and calculation models.

4. Conclusions

In this study, the attenuation properties of 12 different chemotherapy drugs, particularly when exposed to fast neutrons, which are commonly used in cancer treatments, were determined using various calculation methods. It was found that all chemotherapy drugs have a capacity for absorbing neutron radiation when compared to water and paraffin. Notably, Gemcitabine, Etoposide, Vincristine, and Doxorubicin exhibit the highest ΣR values. HVL and λ values were computed using different calculation methods, and Gemcitabine, Etoposide, Vincristine, and Doxorubicin were found to be the chemotherapy drugs closest to water and paraffin. In the study, Oxaliplatin was found to have a lower ΣR value compared to other drugs. These drugs are also administered concurrently with radiotherapy depending on the treatment method. Therefore, knowing and determining their radiation properties will provide an advantage for clinicians.

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
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