

# CURRENT STATUS OF HIGH-ENERGY NEUTRON (14–60 MeV) CROSS-SECTIONS FOR TISSUE KERMA COMPUTATIONS

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## الخلاصة :

إن إستعمال النيوترونات للعلاج الطبي والوقاية يستدعي معرفة معاملات إنطلاق طاقة الحركة في المواد لنيوترونات تصل طاقتها إلى ٦٠ مليون إلكترون فولت . ولكن العقبة في حساب هذه المعاملات وخصوصاً للمواد الأهمية البيولوجية تأتي من نقص المعلومات الدقيقة المتعلقة بمقطع تفاعل النيوترونات مع العناصر الحقيقية . وهذا البحث سيناقش المصادر العالمية للمعلومات النووية المقيمة . وفي حالة عدم وجود معلومات تجريبية متعلقة بمقاطع التفاعلات فإن كثيراً من الباحثين إعتدوا — وبقليل من التوفيق — على نتائج نظرية محسوبة باستخدام نموذج أو أكثر من النماذج المختلفة للنواة (مثل النموذج الضوئي أو النموذج الإحصائي — نموذج التابع النووي الداخلي — نموذج التبخر) . وهذا البحث يقدم متوسط معاملات إنطلاق طاقة حركة النيوترونات في الهيدروجين والكربون والنيوتروجين والأوكسوجين وكذلك في المادة المكافئة لنسيج العضلات . وفي هذا البحث أيضاً سيتم تعريف وتبويب التفاعلات الهامة التي تتعلق بانطلاق طاقة حركة النيوترونات في المواد . وفي هذا الصدد فهناك حاجة ضرورية لمعرفة نتائج تجريبية دقيقة لإحتمال حدوث التفاعلات . وكذلك فهناك نقص كبير في المعلومات التجريبية المتعلقة بإحتمال إنطلاق الجسيمات من مستويات الطاقة في النويات المتبقية . إن طريقة إيجاد معدل الطاقة التي ابتكرها كل من كاسويل وكوين عام ١٩٧٦ مفيدة لحساب طاقة تبيج النواة وكذلك في حساب إحتمال إنبعاث الجسيمات من النواة . ولا بد من التنويه أن معاملات إنطلاق طاقة حركة النيوترونات المحسوبة والتي تتعلق بانبعث جسم معين لا تتفق والنتائج التجريبية وعليه فالنتائج المقدمة في هذا البحث لا يجب الإعتماد عليها في تحديد نوعية النيوترونات .

## ABSTRACT

Neutron kerma factors are required at energies up to 60 MeV for therapy and protection purposes but a major difficulty in their computation for materials of biomedical interest is the lack of sufficiently accurate cross-section data for the light elements. The current situation is reviewed.

World sources of evaluated nuclear data are discussed. Where experimental cross-section information is not available, resort has been made by several authors to calculations using one or more of the standard theoretical models, viz. optical, statistical, intranuclear cascade, evaporation, and phase shift, with limited success. 'Best mean' kerma factors for H, C, N, O, and ICRU muscle tissue are presented.

Those reactions which contribute most to the kerma are identified and tabulated. Good experimental cross-section data are urgently required. There is a dearth of experimental information on the probability of particle emission from excitation levels in the residual nuclei. An energy averaging procedure developed by Caswell and Coyne [22] is useful for evaluating the excitation energy and the probability of particle emission.

Calculated partial kerma factors associated with the emission of a specified particle type are inconsistent with experiment and consequently application of current data to neutron quality specification (e.g. microdosimetry) must be considered unreliable.

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### 1. INTRODUCTION

Kerma factors widely used in neutron dosimetry play the same role as mass energy transfer coefficients ( $\mu_{tr}/\rho$ ) in photon dosimetry, but they are sometimes defined differently because photon fields are traditionally described by energy fluence ( $\chi$ ) whereas neutron fields are usually described by the particle fluence ( $\Phi$ ). The KERMA (kinetic energy released per unit mass of material) [1] is given by:

$$K = \Phi K_f,$$

where  $K_f$  is the kerma factor. For monoenergetic neutron fields of energy  $E_n$ , it is given by

$$K_f = E_n \frac{\mu_{tr}}{\rho}.$$

Kerma factors for various neutron fields have been calculated by several authors [2–20].

### 2. KERMA VALUES

Many neutron beams, in use for radiotherapy, have energies which extend beyond 30 MeV [21]. Therefore kerma values are of profound practical importance in radiation dosimetry for therapy and protection purposes. Accuracy of the available kerma data is limited by the lack of detailed basic nuclear data [22, 23]. Most calculations of kerma are restricted to the neutron energy range < 20 MeV where the most reliable experimental data are available [2–9]. Some authors assume isotropic scattering in the centre-of-mass system.

This assumption becomes increasingly less valid towards higher neutron energies. Nearly all the authors have produced kerma values for materials containing only H, C, N, and O as the kerma factors for some media such as soft tissue, calculated on the basis of an 11-element composition, are equal to the values for the four-element model [5]. In addition there are calculations for media such as bone containing higher atomic number elements which must be taken into account.

Because of the importance in therapy, some authors have attempted to produce kerma values in the neutron energy region > 20 MeV where, however, the

cross-section data are sparse and heavy reliance is placed on theory. Calculations of kerma for neutrons up to 29 MeV, by Caswell and others, [22] were prepared for inclusion in ICRU 26 [24] and subsequently updated [14]. These are based upon experimental neutron cross-section data wherever available (i.e. mainly at lower energy) and, if not, upon application of the nuclear optical model. This method is discussed briefly in Section 4.2 among the more important models which have been adopted by various groups to calculate neutron cross-section data, especially at higher neutron energies where the lack of data is obvious. Alsmiller and Barish [12] and Wells [13] have used an updated version of the so-called ICE model (see Section 4.1) which comprises the intranuclear cascade model of Bertini [25] plus an evaporation phase described by a statistical representation of the probability of particle emission from the excited nucleus. This group of results is extended to 80 MeV and agree best, at lower neutron energies, with the kerma values of Caswell and others [14], although at higher neutron energies the results of both groups for nitrogen are quite different. Dimbylow [15–17] has carried out theoretical calculations of kerma for neutrons in the energy range 20–50 MeV, adopting optical and statistical (Section 4.3) models for calculation of cross-sections, and suggested a method to treat the multi-body break-up reactions at higher energies [26]. The first set of Dimbylow's results [15] agree best with the kerma values of Caswell and others [14] at neutron energies less than 29 MeV.

The various results mentioned above were conflicting in the magnitude of the kerma factors above 14 MeV and led to a reappraisal of the situation by Behrooz [27] and Behrooz and others [18], who used a kinematic approach based on that of Caswell and including allowance for multi-body break-up reactions. All major compilations of cross-section data were re-examined and added to by an independent search of the literature by these authors. These computed kerma factors, which extend to 60 MeV neutron energies, agree best with the lowest of the wide range of values discussed earlier. The latter group of data have been justified by the only experimentally measured kerma values at higher energies [28]. The revised calculation of Dimbylow [16] has produced a set of kerma values in fairly good agreement with the

**Table 1. Averaged Kerma Values ( $\times 10^{-14}$  Gray m<sup>2</sup> n<sup>-1</sup>)\***

$E_n$ (MeV)	H	C	N	O	ICRU muscle tissue
14	$4.712 \pm 0.022$	0.116	0.224	0.170	$0.629 \pm 0.002$
20	$4.690 \pm 0.017$	$0.301 \pm 0.049$	$0.261 \pm 0.062$	$0.194 \pm 0.01$	$0.668 \pm 0.010$
30	$4.444 \pm 0.023$	$0.375 \pm 0.030$	$0.337 \pm 0.069$	$0.265 \pm 0.024$	$0.707 \pm 0.018$
40	$4.193 \pm 0.032$	$0.404 \pm 0.025$	$0.424 \pm 0.077$	$0.319 \pm 0.016$	$0.728 \pm 0.013$
50	$4.047 \pm 0.096$	$0.451 \pm 0.031$	$0.509 \pm 0.069$	$0.368 \pm 0.011$	$0.758 \pm 0.014$
60	$3.834 \pm 0.106$	$0.559 \pm 0.072$	$0.559 \pm 0.063$	$0.432 \pm 0.014$	$0.799 \pm 0.018$

\* Errors are standard deviation of the mean.

lowest set of data. Therefore, Behrooz and Watt [29] have recommended mean values of kerma factors to be applied in radiotherapy and for protection purposes (Table 1). In determining these average values (unweighted) the following subjective adjustments have been made [29]. For hydrogen all data have been included with the exception of the Alsmiller and Barish [12] point at 50 MeV which does not conform with the decreasing trends in kerma with energy expected in theory as is demonstrated in the remaining data. For carbon, nitrogen, and oxygen, the data by Caswell and others [14] have been excluded as this does not include allowance for anisotropic elastic and inelastic scattering. The experimental data of Subramanian and others [28] have been excluded because of the uncertainty in the adjustment factor [29].

A new set of kerma values at neutron energies up to 14 MeV has also been produced by Rubach and Bichsel [20] using cross-section data which were revised by Caswell and Coyne. These are lower values than those obtained by Caswell and others [14].

### 3. NEUTRON CROSS-SECTION DATA

#### 3.1. General Cross-section Data Files

Various extensive compilations of nuclear data are now available. In 1964, the International Atomic Energy Agency (IAEA) established the Nuclear Data Section (NDS) within its Division of Research with the objective of promoting and coordinating the exchange of nuclear data information between its member states. Since 1968 the NDS has been compiling and disseminating evaluated nuclear data (e.g. Evaluated Nuclear Data File (ENDF); United Kingdom Neutron Data Library (UKNDL); German Nuclear Data Library (KEDAK), etc.). In 1970, NDS entered into an

agreement with the other regional data centers (New York, France, Moscow) to share the responsibility of collecting, compiling, and disseminating experimental neutron data and exchanging these in a common computer compatible format. Since that year IAEA has been publishing a computerized index to the literature on microscopic neutron data, called CINDA, on behalf of the regional data centers. In 1974, NDS broadened its programme to include data on charged particle and photo nuclear induced reactions within the scope of its activity. Eventually, in 1976, NDS formed an internationally coordinated network for the systematic compilation, evaluation, and dissemination of nuclear structure and decay data. Within the framework of the IAEA programme, nuclear data means numerical and associated information pertinent to measured, deduced, or calculated parameters of nuclear reactions induced by neutrons, charged particles, and photons, as well as nuclear structure and decay data used in the fundamental and applied nuclear sciences. The most active regional nuclear data center which provides and expands nuclear data files, is the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory, New York, USA, where the ENDF has been provided. This file was the most important source of neutron cross-section data in most of the kerma calculations. The experimentally measured cross-section data are also available through a computerized data storage and retrieval system designed for the transmission of experimental nuclear reaction data between regional nuclear data centers, called EXFOR.

#### 3.2. High Energy Neutron Cross Sections relevant to KERMA

The most extensive up to data information concerning the high energy neutron cross-section data are

**Table 2. Reactions Contributing Most to the Total Kerma in Elemental C, N and O (in %)**

<div><div>Element</div><div><math>E_n</math></div></div>	14 MeV		20 MeV		30 MeV		40 MeV		50 MeV		60 MeV	
Carbon	(n, $\alpha$ )	39.5	(n, n'3 $\alpha$ )	41.4	(n, n'3 $\alpha$ )	62.7	(n, n'3 $\alpha$ )	42.8	(n, n'3 $\alpha$ )	25.8	(n, $\alpha$ npt) $\alpha$	16.2
	elastic	38	elastic	21.5	elastic	10.7	elastic	7.1	(n, dt)2 $\alpha$	8.7	(n, n'3 $\alpha$ )	11.3
	scattering		scattering		scattering		scattering				(n, dt)2 $\alpha$	10.2
	(n, n3 $\alpha$ )	12.5	(n, $\alpha$ )	18.8								
Nitrogen	(n, $\alpha$ )	22.9	(n, n'p)	19.8	(n, dn)	11.7	(n, npn)	13.5	(n, $\alpha$ dn)2 $\alpha$	13.1	(n, $\alpha$ dn)2 $\alpha$	19.1
	elastic	17.3	(n, 2 $\alpha$ )	16.2	(n, npn)	10.8	(n, t $\alpha$ )	9.7	(n, dn $\alpha$ )2 $\alpha$	11.2	(n, npn $\alpha$ )2 $\alpha$	14.5
	scattering		(n, $\alpha$ )	14.9	(n, t $\alpha$ )	10.2	(n, dn $\alpha$ )2 $\alpha$	9.5	(n, nd $\alpha$ )2 $\alpha$	10.1	(n, dn $\alpha$ )2 $\alpha$	9.3
	(n, n'p)	15.3	elastic	14.2	(n, 2 $\alpha$ )	9.4	(n, nd $\alpha$ ) 2 $\alpha$	8.3	(n, npn)	8.9	(n, nd $\alpha$ )2 $\alpha$	8.9
	(n, d)	11.3	scattering						(n, npn $\alpha$ )2 $\alpha$	8.5		
	(n, p)	10.7										
	(n, 2 $\alpha$ )	8.8										
Oxygen	(n, $\alpha$ )	56.3	(n, n' $\alpha$ )	31.7	(n, n'p)	40.6	(n, n'p)	28.5	(n, n2 $\alpha$ )2 $\alpha$	15.9	(n, npnp)	13.1
	elastic	24.5	(n, $\alpha$ )	27.1	(n, n' $\alpha$ )	14.8	(n, n2 $\alpha$ )2 $\alpha$	17.1	(n, npn)	10.1	(n, pnpn)	12.4
	scattering		elastic	15.4			(n, pn)	10.3	(n, pnn)	8.1	(n, pnn)	8.4
			scattering						(n, n'p)	7.8	(n, pn $\alpha$ )	8.3
											(n, n2 $\alpha$ )2 $\alpha$	7.3

given in the proceedings of relevant symposia [30] and also by Behrooz [27], who has extensively reviewed all neutron reactions on H, C, N, and O, and the relevant cross-sections in the energy range 14–60 MeV. All the authors agree on the importance of the contribution of the C(n, n')  $3\alpha$  reaction to kerma in soft tissue. However, Behrooz [27] has indicated that at higher neutron energies (> 30 MeV) the break-up reactions also become important. At neutron energies > 30 MeV about 30% of all the reactions considered produce five or six particles. The contribution of these to kerma at 40, 50, and 60 MeV are 14, 25, and 50.4% respectively for A-150 tissue equivalent plastic.

Reactions making the most important contribution to the total kerma in elemental C, N, and O are listed as percentages of the total kerma in Table 2. However, since analysis of the partial kerma for light particle production reveals serious divergence with experiment [19, 31, 32] one should be wary about applying the present partial cross-section data to, for example, calculation of microdosimetry spectra.

### 3.3 Cross Sections Relevant to Residual Excitation

Lack of enough cross-section data for excitation of various nuclear levels of residual nuclei makes two important problems. One of these is the evaluation of the energy that appears as nuclear excitation leading to  $\gamma$ -ray emission, and is, therefore, not included in the kinetic energy of the charged particles liberated ( $k$ ). This problem produces uncertainty in the total kerma. Secondly, the inadequacy of the cross-section data for

excitation of those nuclear levels which de-excite by emitting charged particles inevitably produces uncertainty in those partial kerma values which are especially important in microdosimetry. There is only very limited measured cross-section data for excitation of nuclear levels. Because of this, a theoretical model, called the Energy Averaging Method, has been employed by Caswell and others [22] to calculate the probability for excitation of various nuclear levels. These authors have mentioned an error of 10% [14] for the method in comparison with the evaluated data of ENDF.

## 4. THEORETICAL MODELS FOR CALCULATION OF CROSS SECTIONS

Various models based upon the properties of nuclei have been developed for calculating the interaction cross-sections. Because of the basic simplifying assumptions, for any single model, one can hope only for an accurate description of a few specific properties and a less detailed representation of the characteristics of some others. It is not surprising then that one may use several models, each of which emphasizes different properties. Some of the more important models which have been used to calculate neutron cross-section data are discussed in the following sections.

### 4.1. Intranuclear Cascade Plus Evaporation Model

Medium energy neutron reaction cross-sections have been successfully described by this model which

is divided into two stages [33]. It is assumed that an incident medium-energy particle interacts with individual nucleons in the target nucleus, rather than by collective interaction, since the time increment during a collision with any individual nucleon is much less than that between intranuclear collisions among the target nucleons. The incident particle and energetic recoil nucleons are assumed to travel through a nucleon gas, interacting only with nucleons encountered in their paths under the restrictions of a nucleon potential and the Pauli Principle. The incident particle may thus pass completely through a nucleus without interaction, or produce an avalanche of nucleon cascades in a period of  $10^{-22}$ – $10^{-23}$  s, some of which may escape the nucleus, while others are absorbed by the nucleus with their energies distributed among the remaining nuclei. At the end of this stage, the residual nucleus is left strongly excited because of its retention of part of the incident particle's energy. The de-excitation of this residual nucleus is accomplished through the evaporation or 'boiling off' of gamma rays, nucleons, and/or clusters of nucleons as massive as  $^{10}\text{Be}$ , in a slower period of  $10^{-13}$ – $10^{-18}$  s.

#### 4.2. Optical model

The optical model derives its name by analogy with the scattering and absorption of light. The presence of a complex optical potential, representing the nucleus, changes the wavelength of nucleons incident on the nucleus and thus provides a macroscopic 'refractive index' for the nucleons. The real part of the complex potential represents scattering and the imaginary part describes nonelastic processes permitted by the Pauli principle and conservation of energy. The imaginary part of the potential causes attenuation of the incident wave. This model is phenomenological in origin and its usefulness lies in its ability to parametrize nuclear data. This model ignores most of the detailed features of nuclear structures and is thus able to give the gross structure of the scattering cross-sections but none of the features that depend on complicated particle states which differ from one nucleus to the next. Thus, the optical model gives cross-sections averaged over resonances, although at higher energies, the resonances become broad. (For more information about this model see Satchler [34].)

#### 4.3. Statistical Model

This model of nuclear reactions is usually based on some assumptions to simplify calculations. In this

method, nuclear reactions can be classified as compound nuclear or direct [34]. In compound nuclear reactions a large number of states in the residual nucleus can be excited with comparable probability, so that the cross-section for excitation of a given nuclear level may be very small. In direct interactions the two systems may make just glancing contact and immediately separate. Their internal states may be unchanged (elastic scattering), one (or both) may be excited by the contact (inelastic scattering), or one or a few nucleons may be transferred across from one nucleus to the other (reaction). In the latter situation, however, the cross-section depends on the matrix element for the interaction taken between the initial and final states of the system. The lower-order process involves a transition between nuclear states that differ in the quantum numbers of only one nucleon. Therefore, the low-lying levels in the residual nucleus are the most strongly excited by the direct interaction. Consequently, at higher energies, the compound nuclear process is the more important mechanism.

#### 4.4. Phase Shift Analysis

In this method a potential is assumed from extrapolation and/or interpolation parameters and an approximate solution of the Schrödinger Equation is calculated using numerical techniques. Alternatively one may extrapolate from or interpolate among parameters of the functional representation of the solutions to the Schrödinger Equation. The wavefunction of elastically scattered neutrons may be expressed in terms of angular functions (such as Legendre polynomials). Accordingly the observed angular distribution characteristics are produced [35, 36].

### 5. CONCLUSION

The wide spread in the kerma values calculated by different groups indicates a need for more accurate and intensive cross-section data, since the main sources of uncertainty in such calculations are the uncertainties in the available nuclear data and errors introduced by estimating data which have not yet been measured. In general, the available data have uncertainties varying from a few percent (for hydrogen elastic scattering) to 20% at lower energies and to about 40% at higher energies. Even when data are available, its separation into partial interaction cross-sections is usually not and therefore one has to calculate these using a model. Consequently a much larger uncertainty will appear (often about 20 to 50%). If only sparse nuclear data are

available, the uncertainties are large. Generally at higher energies the cross-sections become increasingly unpredictable. It is not feasible to recommend any single model for calculation of cross-section data because each model is intended for application only in certain energy bands and for certain elements. Therefore, the uncertainties in kerma factors are dependent on the cross-sections and the energy range and vary from element to element. To improve the accuracy of calculated kerma factors, the need for more and better cross-section data, especially at neutron energies greater than 20 MeV, is obvious. Below 20 MeV a more detailed evaluation of available data and more partial interaction cross-section data are urgently required. Kerma factors at neutron energies higher than 30 MeV are more sensitive to multi-body break-up reactions. Therefore, to obtain more accurate results, the measurement of these reaction cross-sections is highly desirable. Finally, it is necessary to explore quantitatively the role of the discrete excitation levels from both the experimental and theoretical standpoints, as the partial interaction and differential cross-sections are largely unknown.

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