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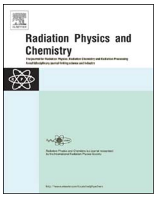

Comparison of the neutron ambient dose equivalent and ambient absorbed dose calculations with different GEANT4 physics lists

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ABSTRACT

A comparison between neutron physics lists given by GEANT4, is made in the calculation of the ambient dose equivalent, and ambient absorbed dose, per fluence conversion coefficients ($H^{*}(10)/\phi$ and $D^{*}(10)/\phi$) for neutrons in the range of 10^{-9} MeV to 15 MeV. Physics processes are included for neutrons, photons and charged particles, and calculations are made for neutrons and secondary particles. Results obtained for QBBC, QGSP_BERT, QGSP_BIC and Neutron High Precision physics lists are compared with values published in ICRP 74 and previously published articles. Neutron high precision physics lists showed the best results in the studied energy range.

1. Introduction

The international system of radiation protection is based upon the definition by both the International Commission of Radiation Units and Measurements (ICRU) (ICRU, 1993) and the International Commission of Radiation Protection (ICRP) (ICRP, 2007) of protection quantities, such as the effective dose E and the tissue equivalent dose H_T that relate to stochastic and deterministic health effects and the measurement of operational quantities such as the personal dose equivalent H_p(d) and the ambient dose equivalent H*(d) which should be overestimates of the protection quantities and can be measured by individual dosemeters and area monitors.

Fluence to dose equivalent conversion coefficients provide the basis for the calibration of area and personal monitors. The ICRP in its report 74 (ICRP, 1996) publishes tables of fluence to ambient dose equivalent conversion coefficients for photons and neutrons obtained by Monte Carlo simulation. Different codes were used in the calculations, including MCNP (Los Alamos National Laboratory, 2016). MCNP is one of the most used Monte Carlo codes and having been benchmarked for an extensive range of neutron energies, in different applications, it is the usual choice for neutron simulations. MCNP is distributed by the RSICC (Radiation Safety Information Computational Center, 2017) under customer demand which, if approved, requires the user to provide specific information to RSICC and agree to certain terms and conditions before being granted access to the system.

An open source alternative to MCNP is GEANT4 (GEometry ANd Tracking) (GEANT4, 2016; Allison et al., 2016), a Monte Carlo toolkit for simulating the passage of particles through matter. It is freely available from CERN (the European Organization for Nuclear Research), and maintained by a collaboration composed of a sizeable international research organization formed by individuals from a number of cooperating institutes, HEP experiments, and universities (Agostinelli et al., 2003). Presently, GEANT4 can be used in a huge variety of experiments and projects including high energy physics, astrophysics and space science, medical physics and radiation protection. Its functionality and modelling capabilities continue to be extended, while its performance is enhanced (Allison et al., 2006). This work focus on the calculation of fluence to ambient dose equivalent conversion coefficients for neutrons using the Monte Carlo toolkit GEANT4.

Having been developed for high energy physics simulations, GEANT4 has been extensively tested for neutron physics above 100 MeV (Allison et al., 2016). Santoro et al. (2016), tested the GEANT4 performance for the fast neutron generation mechanism by thermal neutron capture in ^{6}Li. Thermal neutron capture on different targets has been studied by Enger and Ende (Ende et al., 2016; Enger et al., 2006). Ende tests GEANT4 for detailed boron-lined neutron detector characterization benchmarking it against MCNPX. Enger calculated thermal neutron capture in gadolinium comparing MCNP and GEANT4 results with experimental data. However, the version of GEANT4 (6.0) used in this work did not include thermal neutron scattering from chemically bound atoms and the authors concluded that GEANT4 was not a reliable code for low energy neutron dosimetric calculations in medical applications such as Neutron Capture Therapy (NCT). This type of scattering was incorporated in version 8.2 of GEANT4 and Garny et al. (2009) compared results of ambient dose

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equivalent for neutrons with MCNP and values published in ICRU report 57 (ICRU, 1998). Geng et al. (2015) investigated depth dose distributions (homogeneous phantom), and fluence-to-dose conversion coefficients for different organs (Chinese hybrid male phantom) comparing the calculated results with MCNP5.

Having been developed for such a wide range of particles and energies, the toolkit offers the user a number of different physics lists that should be chosen according to the particular problem to be tackled. For radiation protection applications, that usually deal with energies of the order of keV or a few MeV, for photons and neutrons, the so-called High Precision physics lists are recommended.

As a means of comparison between neutron physics lists for our study, the neutron ambient dose equivalent, H*(10) was used. H*(10) is a weighted radiation dose which takes the quality factor of the particles depositing energy in biological matter into account. The quantity ambient absorbed dose, denoted as D*(10) by the (ICRU, 1993) is also included in this comparison. D*(10) is obtained by calculating the absorbed dose inside the ICRU sphere, at a depth of 10 mm, without using any quality factor. In this study the H*(10) calculations were performed using version 10.1 of GEANT4 and the results were compared with the ICRP results for energies ranging from 10^{-9} MeV to 15 MeV. The ambient absorbed dose, D*(10), was compared with previous publications (Leuthold et al., 1992; Veinot and Hertel, 2005).

2. Materials and methods

2.1. Neutron physics lists

GEANT4 version 10.1 was used running on Ubuntu 14.04.2 LTS. The physics lists recommended by the GEANT4 Collaboration to simulate particle transport problems including neutrons are QGSP_BERT_HP, QGSP_BIC_HP, QGSP_BERT, QGSP_BIC and QBBC (Agostinelli et al., 2003) of which the High Precision ones adopt the same neutron package to describe neutron interactions from thermal energies up to 20 MeV and henceforth will be denoted as GEANT4_HP in this paper. An additional physics list denoted by GEANT4_HP_T was defined in this work to study the scattering of neutrons with energies below 4 eV. Each physical process was then chosen individually for each particle. This GEANT4_HP_T thermal physics list takes the chemical binding and crystal structure into account by using S(α,β) data. This is needed for calculations of thermal neutron scattering on molecules such as water and polyethylene.

G4NDL is a data set containing files for high precision neutron model cross section data when the neutron energy is below 20 MeV. These data come largely from the ENDF/B-VI library which is developed and maintained by the Cross Section Evaluation Working Group (CSEWG) (Herman, 2016). Other evaluated data are produced using the G4NDL data set via averaging procedure for neutron energies $E < 10$ MeV. For energies $E > 20$ MeV the cross-sections are computed by Geant4 cross-section classes G4BGGNucleonInelasticXS and G4BGGNucleonElasticXS. For the interval $E = 10–20$ MeV a linear interpolation is used (Credit/citations for data files, 2016).

Tables 1, 2 list the processes with their related models and cross-sections informations of all physics lists used in the present work.

Table 2
Models and their related cross sections.

Model	Cross Section
NeutronHPElastic	NeutronHPElasticXS
NeutronHPInelastic	NeutronHPInelasticXS
NeutronHPCapture	NeutronHPCaptureXS
NeutronHPFission	NeutronHPFissionXS
NeutronHPThermalScattering	NeutronHPThermal- ScatteringData
hElasticCHIPS	ChipsNeutronElasticXS (QGSP_BERT and QGSP_BIC G4NeutronElasticXS (QBBC)
BertiniCascade	G4NeutronInelasticXS
nRadCapture	G4NeutronCaptureXS
BinaryCascade	G4NeutronInelasticXS

Table 1
Neutron physics lists in GEANT4 for energies below 20 MeV.

Process	**Physics List**				
	GEANT4_HP	GEANT4_HP_T	QGSP_BERT	QGSP_BIC	QBBC
Elastic	NeutronHPElastic	NeutronHPThermal- Scattering (0–4 eV) NeutronHPElastic (4 eV–20 MeV)	hElasticCHIPS (ChipsNeutron-ElasticXS)	hElasticCHIPS (ChipsNeutron-ElasticXS)	hElasticCHIPS (G4Neutron-ElasticXS)
Inelastic	NeutronHPInelastic	NeutronHPInelastic	BertiniCascade	BinaryCascade	BinaryCascade
Capture	NeutronHPCapture	NeutronHPCapture	nRadCapture	nRadCapture	nRadCapture
Fission	NeutronHPFission	NeutronHPFission	N/A	N/A	N/A

Electromagnetic interactions were considered in all physics lists used. QGSP_BERT, QGSP_BIC, QBBC and GEANT4_HP use the GEANT4 standard electromagnetic physics.

GEANT4_HP_T uses the G4EmLivermore model for electromagnetic interactions. All ion interactions are described by G4ionIonisation, G4HadronElastic and G4MultipleScattering. G4hIonisation was used for some special ions asdeuterons and alphas. Besides these, we used G4HadronInelasticProcess, G4ProtonInelasticProcess and G4AlphaInelasticProcess.

2.2. Geometry configuration

The ICRU sphere was implemented in GEANT4 version 10.1. The sphere has a radius of 15 cm and it is made of tissue-equivalent (TE) material. The composition and physical quantities are given in Table 3.

The starting neutrons were produced uniformly in a disc surface configuration with the same radius of the sphere. In order to score the ambient dose equivalent, a cylindrical volume (10 mm diameter, 2 mm height) was placed 10 millimeters deep inside the sphere. The scoring has the same TE-material as the ICRU sphere and it was located with the circular cross section facing the incoming beam (see Fig. 1). All the simulation occurs in a world volume ($1 \times 1 \times 1$ m^3), where the space is filled with vacuum (very low density air, density of 10^{-25} g/cm^3).

The conversion coefficients H*(10)/ϕ and D*(10)/ϕ were calculated for fifteen neutron energy values in the range of 10^{-9} to 15 MeV.

2.3. Quality factor and ambient dose equivalent calculations

As neutrons interact with the material medium, they produce secondary charged particles that loose energy until they come to rest. As the quality factor of a secondary charged particle depends on the linear energy transfer (LET) and the LET depends on the particle energy, the ambient dose equivalent should be calculated continuously by multiplying the absorbed dose by the corresponding quality factor along the particle path. In the simulation, the energy loss happens in each of the particle steps and most of the times, the particle loses all of its energy in a single step. For those particles, the information on the

Table 3
Determination of tissue equivalent (TE) material in GEANT4.

Element	Percent (%)	Physical quantities
Oxigen	76.2	temperature = 300 k
Carbon	11.1	density = 1.0 g/cm^3
Hidrogen	10.1	
Nitrogen	2.6	

[a]Composition given in mass fraction

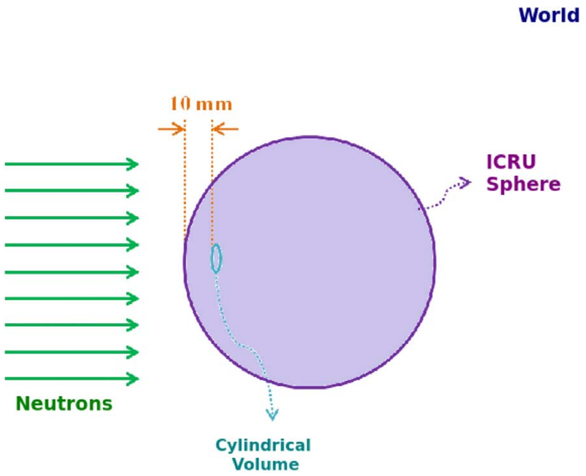

Fig. 1. ICRU sphere. Geometry used for $H^*(10)/\phi$.

intermediary energies is not available to the simulation. For this reason, a mean quality factor was calculated to simulate the slowing down of the charged particle. The required stopping power data (LET(E)) were taken from ICRU 49 (proton and alpha) (ICRU, 1993) and ICRU 73 (heavy ions: C, N and O) (ICRU, 2005), and to each LET value a Q value was assigned according to the Q(L) relationship from ICRP 60 (ICRP, 1991).

$$Q = \begin{cases} 1 & L < 10\frac{keV}{\mu m} \\ 0.32L - 2.2 & 10 \le L \le 100\frac{keV}{\mu m} \\ 300/\sqrt{L} & L \ge 100\frac{keV}{\mu m} \end{cases} \tag{1}$$

Then, Q_{mean} is calculated by Eq. (2). The mean quality factor was calculated for protons, alphas, ^{12}C, ^{14}N and ^{16}O, and the difference between both pointwise and mean quality factors has been shown by Garny et al. (2009).

$$Q_{mean}(E_{start}) = \frac{\int_{E_{start}}^{0} Q(LET(E))dE}{\int_{E_{start}}^{0} dE} \tag{2}$$

For each charged secondary particle created in the sensitive volume, let D_{total} be the total absorbed dose in the volume due to that particle. Considering that the particle loses all its energy in that volume, then $D_{total} = E_{start}/m$ where m is the mass of the sensitive volume and E_{start} is initial particle energy. If $Q_{mean}(E_{start})$ is the mean quality factor of particles with initial energy E_{start}, then H*(10) is defined by Eq. (3).

$$H^*(10) = \sum_{particles} Q_{mean}(E_{start}).\ D_{total} \tag{3}$$

The fluence of neutrons inside the sphere was obtained by a track length estimator and the ambient dose equivalent per unit fluence conversion coefficient, $H^*(10)/\phi$, was calculated for some neutron energies and compared with results from ICRP 74.

3. Results and discussion

In order to verify the feasibility of applying GEANT4 code for neutron calculations in radiation protection, the ambient dose equivalent was calculated, as well as the ambient absorbed dose. GEANT4 physics lists were tested over an energy range from 10^{-9} to 15 MeV. The results of GEANT4 physics lists were compared to each other, with ICRP 74 and previously published results.

The ambient dose equivalent per neutron fluence ($H^*(10)/\phi$) and the ambient absorbed dose per neutron fluence ($D^*(10)/\phi$) are presented in Figs. 2 and 3. The uncertanties of QGSP_BERT, QGSP_BIC and QBBC are smaller than 1% for k = 2 and they are not represented in the figures. The ICRP 74 results are presented in the figure with ± 10% uncertainty margin arising from calculations in this report.

For neutron energies above 1 MeV, all the physics lists in GEANT4 show good agreement with the ICRP report ambient dose equivalent values. When the neutron energy is below 1 MeV, the conversion coefficients $H^*(10)/\phi$ obtained with QGSP_BERT and QGSP_BIC begin to show significant deviations towards lower values than those in the report. A discrepancy can be observed in QBBC physics, for energies below 1×10^{-2} MeV. For energies below this value, only the GEANT4_HP and GEANT4_HP_T physics lists show consistency with

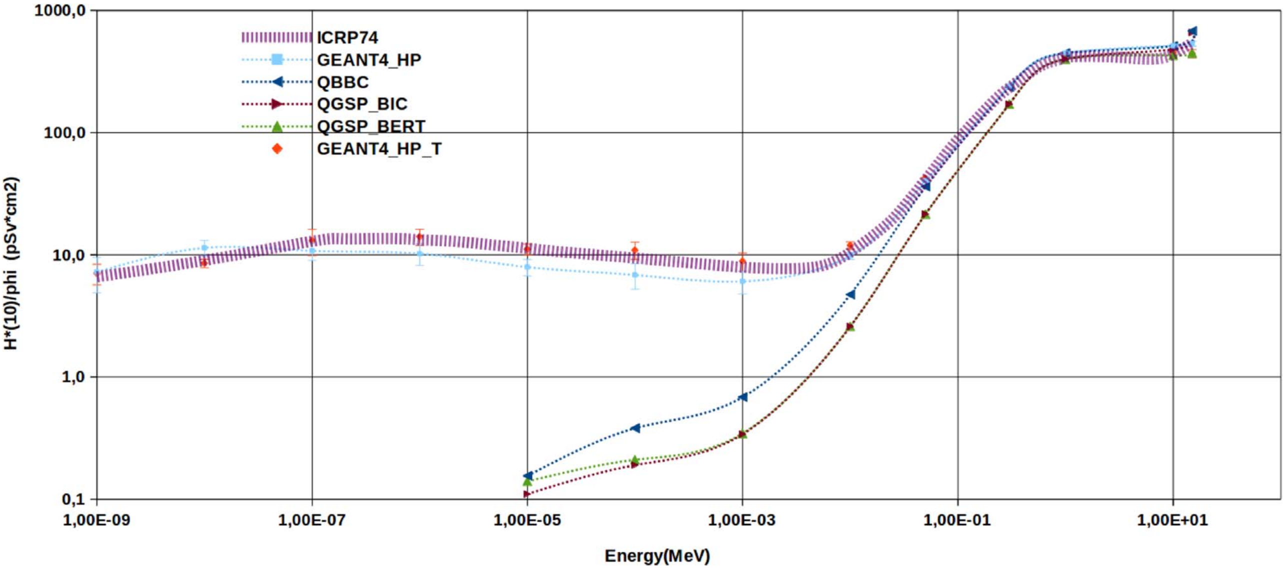

Fig. 2. Comparison of different physics lists for ambient dose equivalent calculations H*(10)/ϕ.

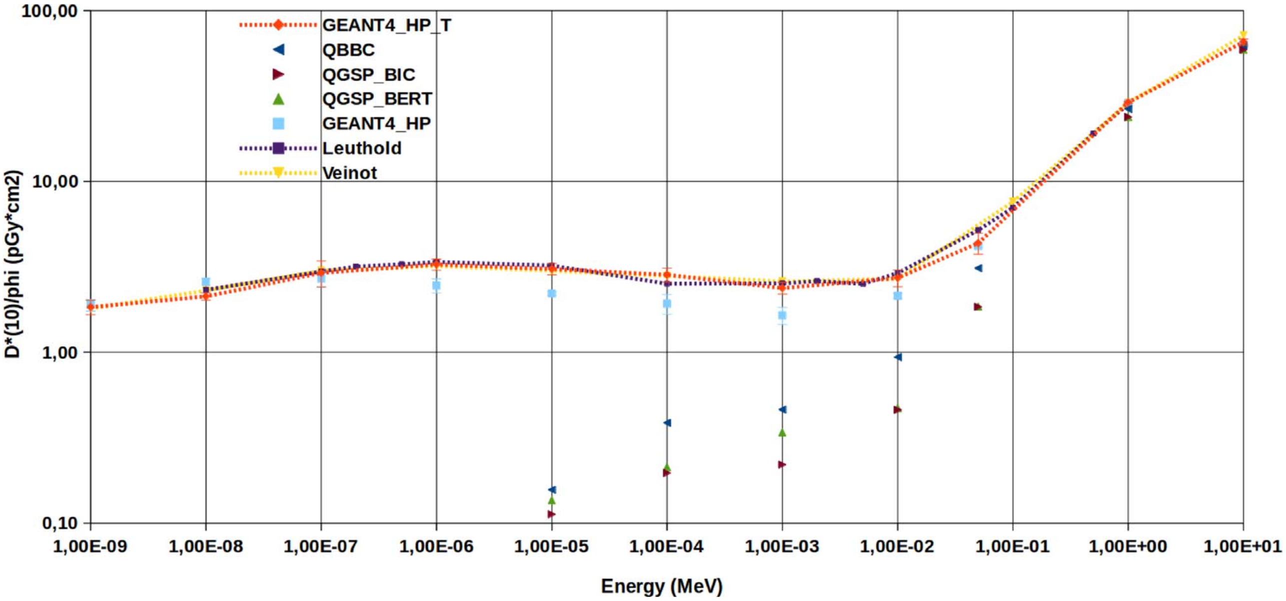

Fig. 3. Comparison of different physics lists for ambient dose D*(10)/ϕ.

the ICRP results. QGSP_BERT, QGSP_BIC and QBBC fail to obtain ambient dose equivalent or ambient dose results in GEANT4 for energies below 1×10^{-5} MeV. Within the uncertainties, GEANT4_HP agrees with the reference for energies equal to or below 1×10^{-7} MeV and underestimates the reference for energies between 1×10^{-6} and 1×10^{-3} MeV. GEANT4_HP_T is the only physics list that shows good agreement with the ICRP values within the uncertainties for all range of energies. That is attributed to the inclusion of the scattering matrix S (α,β) to the physics, which is not done in the other cases. These results suggest that for incident neutron energies below 1×10^{-3} MeV a correct treatment of thermal neutrons propagation is needed for the correct evaluation of H*(10).

Results for $D^*(10)/\phi$ in GEANT4 were compared to references (Leuthold et al., 1992; Veinot and Hertel, 2005). Both of them used MCNP for their calculations. In general, these results follow the same behaviour as the $H^*(10)/\phi$. QGSP_BERT, QGSP_BIC and QBBC physics lists underestimate the references below 1×10^{-1} MeV and should not be used for dosimetric calculations. GEANT4_HP underestimates the reference values for energies between 1×10^{-6} and 1×10^{-2} MeV. The maximum discrepancy found between GEANT4_HP_T and Leuthold et al. (1992) is 16% of the reference value at the energy of 5×10^{-2} MeV. When compared to Veinot and Hertel (2005), the highest difference is 9% at 10^{-3} MeV.

Even with the same physics model (see Table 1), QGSP_BIC and QBBC have different conversion coefficients results. This can be explained by their different cross sections (Table 2) for the elastic scattering processes, which are important for neutrons in this range of energy. The same can not be said about inelastic scattering processes and this is proved by the identical results from QGSP_BERT and QGSP_BIC (Fig. 2), which have similar elastic models and cross sections, but different inelastic models. Consequently, the similar results are caused by the use of the same elastic scattering models.

3.1. Uncertainty analysis

The number of primary histories was set to 1×10^{9} for all the physics lists, except GEANT4 high precision ones, which was set to 4×10^{8}. This was chosen because HP (with and without thermal option) package are extremely time consuming. Therefore, four processes were run with different seeds and an average was taken from the runs. The standard deviation was calculated to this average. The same was generated to high precision with thermal scattering correction. The other physics lists were less time consuming than the HP ones, enabling a number of 1×10^{9} primary histories, decreasing the simulation error. In the calculations of H*(10), a maximum uncertainty of 24% within 2 sigma was obtained for the GEANT4_HP_T physics list at 1×10^{-7} MeV. For D*(10), a maximum uncertainty of 18% within 2 sigma was obtained for the GEANT4_HP_T physics list at 1×10^{-7} MeV.

4. Conclusion

In this work, we compared the physics lists recommended by GEANT4 to calculate neutron transport (GEANT4_HP, GEANT4_HP_T, QGSP_BERT, QGSP_BIC and QBBC). For this, simulations of neutrons of energies between 1×10^{-9} and 15 MeV were performed to calculate ambient dose equivalent per fluence (H*(10)/ϕ) and the ambient absorbed dose per fluence (D*(10)/ϕ) conversion coefficients. Results of all physics lists were compared to ICRP 74 and previously published works.

QGSP_BERT, QGSP_BIC and QBBC show good agreement with ICRP at high energies (QBBC above 1×10^{-2} MeV and QGSP_BERT and QGSP_BIC for energies above 1 MeV) and present no dose results for energies below approximately 1×10^{-5} MeV.

The neutron high precision physics lists proved to be the best choice for the range studied in this work and their results agree well with ICRP 74. A refinement of the high precision results is obtained by applying a specific treatment for thermal neutrons elastic scattering from chemically bound atoms. This correction is necessary for a precise evaluation of H*(10)/ϕ when the incident neutron energy is below 1×10^{-3} MeV.

In particular, for medical applications, it was not clear until now if Geant4 was suitable for dosimetric calculations such as Neutron Capture Therapy. This work shows that the present status of the code allows its use in this area provided that the thermal neutrons elastic scattering treatment is considered in the user defined physics list. Furthermore, we show that GEANT4 can also be used for neutron dose calculations for radiation protection purposes where the interaction of thermal neutrons with human tissue is important such as in voxel phantoms and in the calibration of personal and area dosemeters in terms of the quantities H*(10) and Hp(10).

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