

# The influence of nuclear models and Monte Carlo radiation transport codes on stray neutron dose estimations in proton therapy

M. De Saint-Hubert<sup>1\*</sup>, J. Farah<sup>2</sup>, M. Klodowska<sup>3</sup>, M. T. Romero-Expósito<sup>4,5</sup>, K. Tyminska<sup>6</sup>, V. Mares<sup>7</sup>, P. Olko<sup>8</sup>, L. Stolarczyk<sup>8,9</sup> and S. Trinkl<sup>10</sup>

<sup>1</sup> Belgian Nuclear Research Centre (SCK CEN), Boeretang 200, BE-2400 Mol, Belgium.

<sup>2</sup> Institut de Radioprotection et de Sûreté Nucléaire (IRSN), Pôle Radioprotection de l'Homme, BP17, 92260 Fontenay-aux-Roses, France.

<sup>3</sup> Department of Medical Physics and Clinical Engineering, Addenbrooke's Hospital, Hills Road, Cambridge, CB2 0QQ, United Kingdom.

<sup>4</sup> Universitat Autònoma de Barcelona, Departament de Física, E-08193 Bellaterra, Spain.

<sup>5</sup> Instituto Tecnológico de Santo Domingo (INTEC), P.O. Box 342-9/249-2, Santo Domingo, República Dominicana.

<sup>6</sup> National Centre for Nuclear Research, A. Soltana 7, 05-400 Otwock-Swierk, Poland.

<sup>7</sup> Helmholtz Zentrum München, Institute of Radiation Medicine, Ingolstädter Landstraße 1, 85764 Neuherberg, Germany.

<sup>8</sup> Institute of Nuclear Physics PAN, Radzikowskiego 152, 31-342 Krakow, Poland.

<sup>9</sup> The Danish Centre for Particle Therapy, Aarhus University Hospital, Palle Juul-Jensens Boulevard 25, DK-8200 Aarhus, Denmark.

<sup>10</sup> Federal Office for Radiation Protection, Medical and Occupational Radiation Protection, Ingolstädter Landstraße 1, 85764 Neuherberg, Germany.

\*corresponding author: [mdsainth@sckcen.be](mailto:mdsainth@sckcen.be)

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30 **Abstract**

31 **Purpose:** This study investigates the influence of several Monte Carlo radiation transport codes and  
32 nuclear models on the simulation of secondary neutron spectra and its impact on calculating and  
33 measuring the neutron doses in proton therapy.

34 **Materials and methods:** Three different multi-purpose Monte Carlo radiation transport codes  
35 (FLUKA, MCNPX, Geant4) were used together with different available nuclear models, to calculate  
36 secondary neutron energy spectra at various points inside a water tank phantom with PMMA walls  
37 using a 10 x 10 cm<sup>2</sup> rectangular, mono-energetic proton beam (110 MeV, 150 MeV, 180 MeV, 210  
38 MeV). Using Kerma approximation secondary neutron doses were calculated applying fluence-to-  
39 dose equivalent conversion coefficients in water. Moreover, the impact of varying spectra for  
40 electrochemically etched CR39 detector calibration was analyzed for different codes and models.

41 **Results:** In distal positions beyond the Bragg peak, results show largest variations between the codes,  
42 which was up to 53% for the high energy neutron fluence at 16 cm from the Bragg peak of the 110  
43 MeV proton beam. In lateral positions, the variation between the codes is smaller and for the total  
44 neutron fluence within 20%. Variation in the nuclear models in MCNPX was only visible for the proton  
45 beam energies of 180 and 210 MeV and modeling the high energy neutron fluence which reached  
46 up to 23% for 210 MeV at 11 cm lateral from the beam axis. Impact on total equivalent dose was  
47 limited for the different models used (<8%) while it was pronounced for the different codes (45% at  
48 16 cm from the Bragg peak of the 110 MeV proton beam). CR39 calibration factors in lateral positions  
49 were on average varying 10% between codes and 5 % between nuclear models.

50 **Conclusions:** This study demonstrated a large impact on the neutron fluence spectra calculated by  
51 different codes while the impact of different models in MCNPX proved to be less prominent for the  
52 neutron modeling in proton therapy.

53 **Keywords:** Monte Carlo radiation transport codes, nuclear models, neutron dosimetry, CR39, proton  
54 therapy.

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**Highlights:**

- Monte Carlo code and nuclear model impact neutron spectra, dose and CR39 calibration
- Codes have larger neutron spectra variation in distal versus lateral positions
- Impact of MCNPX neutron model is only visible for 180 MeV and 210 MeV proton beams
- Calculated total dose equivalent varied up to 45% between the codes
- CR39 calibration factors varied within 10% and 5% between codes and nuclear models

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66 **Introduction**

67 In recent years, major technological breakthroughs allowed for more compact and affordable proton  
68 therapy units further increasing the number and popularity of such facilities worldwide with more  
69 than 66 systems in operation in 2020 and 31 under construction. The physical behavior of protons  
70 result in a sharply localized peak of dose, known as the Bragg peak, allowing improved target dose  
71 conformation, with reduced entrance and negligible exit dose when compared to other radiotherapy  
72 techniques [1]. Nevertheless, one of the challenges of proton therapy is the production of secondary  
73 neutrons which are unavoidable due to nuclear interactions of high energy protons with beam line  
74 materials and with the patient’s body [2]. As therapeutic proton beams have energy of hundreds of  
75 MeV and interact with materials of different tissue compositions and densities secondary neutrons,  
76 with energies from thermal to high-energy, are inevitably encountered during particle therapy.

77 Currently, none of the available neutron counters and detectors is fully compatible with a clinical  
78 measurement of neutron spectra inside the patient or within an anthropomorphic phantom. Hence,  
79 many studies strongly rely on Monte Carlo (MC) particle transport calculations, which are often  
80 considered as the reference. The literature extensively reports the use of multiple purpose MC codes  
81 such as FLUKA [3-5], MCNPX [6], GEANT4 [7] and PHITS [8] for several applications in proton therapy.  
82 First of all, MC codes can be used for out-of-field dosimetry as it allows to compute neutron doses  
83 [9-11], which are not considered by the current treatment planning systems used in PT. Furthermore,  
84 the shielding of proton therapy facilities is often based on results from MC simulations which allow  
85 the computation of neutron ambient dose equivalent [12-14] and the spectral neutron fluence inside  
86 and outside the treatment room [15-19].

87 Only few studies have compared MC simulations to experimental measurements of neutron doses,  
88 ambient dose equivalents and Bonner sphere spectrometry in proton therapy (PT) [16, 19-24]. Such  
89 studies highlighted large discrepancies between experimental results and MC simulations with up to  
90 factors 2-3 presumably due to large measurement uncertainties as well as limitations of nuclear  
91 reaction models and cross sections integrated into the MC codes. In general, MC codes allow accurate  
92 calculations for neutrons below 20 MeV thanks to existing and well evaluated data libraries, such as  
93 ENDF/B [25, 26], which provide reliable neutron cross section data. Above 20 MeV cross-section data  
94 are scarce or non-existing for several materials and MC codes. Up to 150 MeV neutrons, MCNP has

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95 the ability to utilize data libraries that have recently been released by LANL Group T-2 [27].  
96 Nevertheless, some codes do not use these cross-sections for higher energies and need to rely on  
97 nuclear models that describe the interaction of protons and neutrons with target nuclei. Several of  
98 these models are available such as Intranuclear Cascade (INC) models (e.g. Bertini, Binary INC model,  
99 ISABEL model), pre-equilibrium models as well as evaporation models (e.g. Dresner and Abla). In  
100 general, it is difficult to define which of the models are more suitable for simulations in a particular  
101 application and for specific elements.

102 Benchmarking studies have been conducted for heavier elements such as copper and iron [28, 29]  
103 but not yet for light elements constituting biological tissues such as hydrogen, oxygen, nitrogen,  
104 carbon. Moreover, the influence of MC codes and selection of nuclear models have been tested for  
105 Bonner sphere spectrometry (BSS) measurements, as BSS require the input of an initial guess  
106 spectrum to start the unfolding process. It was shown that secondary neutron doses from cosmic  
107 irradiation as measured with BSS have an uncertainty of 10% related to the different nuclear models  
108 and transport codes (GEANT4 and MCNP) [30]. More recently, an even more extended  
109 intercomparison of codes (MCNP, MCNPX, FLUKA, PHITS, MARS, or GEANT4) showed an uncertainty  
110 of unfolded neutron fluences above 20 MeV of about 20% [31]. Not only BSS and rem counters  
111 require MC simulations to assess pre-requisite information for its calibration, also passive detector  
112 systems may require MC for energy response correction and/or appropriate calibration. For example,  
113 the calibration of electrochemically-etched track detectors (CR39) and the conversion of track  
114 density into dose rely on a fluence factor, which is often estimated through MC simulations for a  
115 predefined standard neutron source [32, 33] The accuracy and consistency of MC simulations may  
116 hence affect experimental measurements by expanding their associated uncertainties and adding up  
117 a major component which is currently not quantified.

118 The European Radiation Dosimetry Group working group 9 (EURADOS WG9) research focusses on  
119 the assessment of neutron ambient dose in the proton treatment room and in the facility [34-36] as  
120 well as in the patient, more specifically assessing the undesired out-of-field doses during proton  
121 therapy [37-39]. Several types of ambient monitors as well as numerous passive detector types have  
122 been studied and compared for stray radiation using water and anthropomorphic phantoms. Also  
123 comparison of experimental data to MC calculations is often performed, involving the use of many

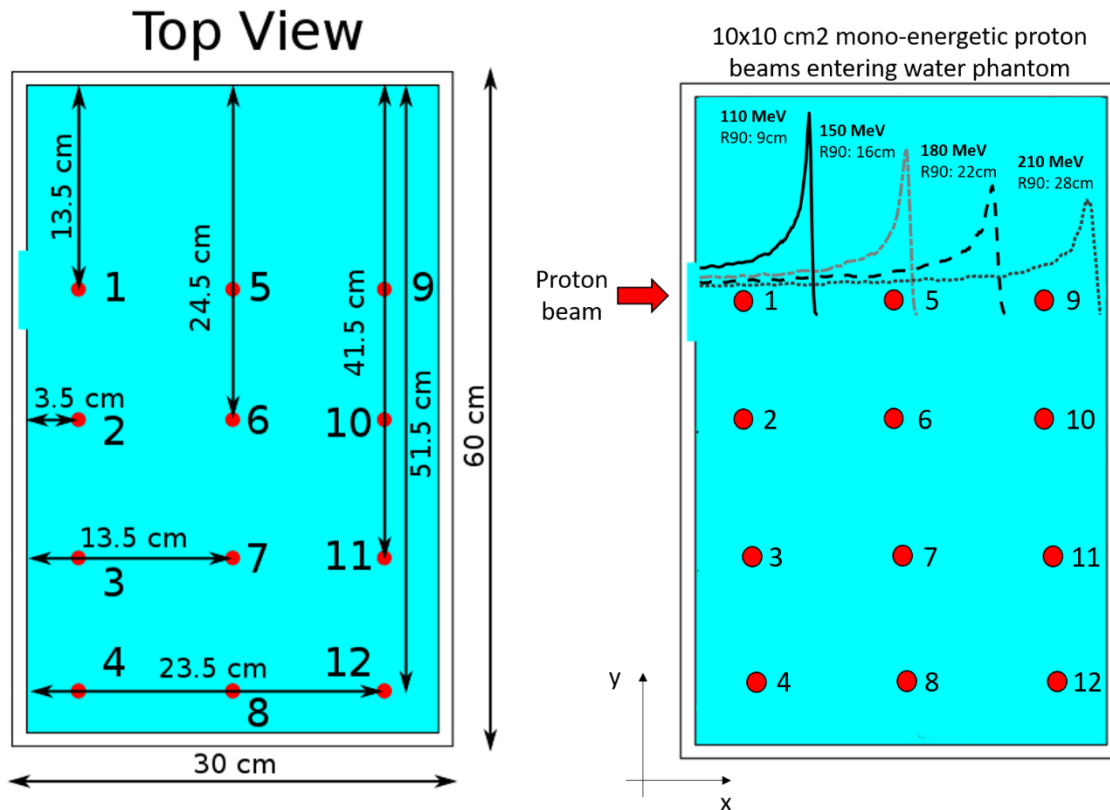
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124 different MC codes and models. Nevertheless, an intercomparison of the different available Monte  
125 Carlo codes is missing and needed to assess their performance, identify limitations as well as its  
126 impact on the experimental data. This study focused on comparing three widely used MC codes,  
127 FLUKA, MCNPX and GEANT4, in the prediction of secondary neutrons following nuclear reactions of  
128 a typical proton therapy beam with light elements. The work first involved modeling of a large  
129 experimental campaign performed by WG9 [36, 37]. The MC codes were first compared to check  
130 their accuracy in reproducing the therapeutic pencil proton beam targeting a 30 x 60 x 30 cm<sup>3</sup> water  
131 tank phantom. Next, simulations of neutron spectra inside the water tank phantom were performed  
132 at different depths and lateral positions with respect to the Bragg peak and the different fluences  
133 were compared. Finally, the variability of neutron spectra among the codes and their impact on  
134 experimental measurements was assessed for electrochemically etched CR-39 detectors used in  
135 previously conducted experimental campaign [36, 37]. The spectra are needed to determine the  
136 calibration factor because in electrochemically etched CR-39 detectors the size of a track does not  
137 depend on neutron energy [33].

## Materials and Methods

### Water phantom and beam parameters

A 30 x 60 x 30 cm<sup>3</sup> water phantom with polymethyl methacrylate (PMMA) wall thickness of 15mm and a beam entrance wall with thickness of 4 mm (area 12 x 12 cm<sup>2</sup>) was modelled as shown in figure 1. This water phantom was developed by Bordy, et al [40] and used during previously conducted experimental studies within EURADOS WG9 [36, 37]. To investigate the influence of nuclear models on MC particle transport calculations a simple beam model was implemented with four different proton energies of 110 MeV, 150 MeV, 180 MeV and 210 MeV. A 10 x 10 cm<sup>2</sup> rectangular parallel beam of mono-energetic protons was modelled entering the water phantom at the beam entrance window. Outside the water phantom the beam was travelling through 50 cm of air.



**Figure 1.** On the left a schematic representation of the 30 x 60 x 30 cm<sup>3</sup> water phantom with PMMA walls of 15 mm consisting of a beam entrance window with a thickness of only 4 mm (area 12 x 12 cm<sup>2</sup>) and 12 different positions (1cm diameter spheres) used for the calculations performed with the different MC simulation codes/models. On the right the entrance of the parallel rectangular 10x10 cm<sup>2</sup> proton beams indicated with

an arrow including Bragg curves for the respective proton energies (MCNPx) demonstrating their different ranges (R90 values) and positions towards the 12 positions in the water phantom.

First, the depth dose distribution for all the four mono-energetic beams was scored using voxelization of the water phantom, with voxel sizes of 1 mm<sup>3</sup>. For the definition of range the 90% dose in the distal falloff (R90) values were calculated and we report in this manuscript on the interpolated R90 values for each energies. The distance refers to the distance inside the water phantom (outer wall is set to position zero), thus including a 4mm PMMA wall followed by water (see figure 1).

Furthermore we defined several positions inside the water phantom. In total 12 different positions were defined for comparison of neutron spectra, neutron dose equivalent and CR39 calibration factor. This involved spherical tally volumes of 1 cm diameter (see figure 1).

**Table 2.** Overview of relative positions towards proton beams for the different mono-energetic proton beams in position 1, 5, 9, 2, 6 and 10. In bold positions that we consider out-of-field, i.e. not within the proton beams Bragg curve. Between brackets the distance towards the Bragg peak (R90) isocenters (0,0) in x and y coordinates as indicated in figure 1.

Positions	Mono-energetic proton beams			
	110 MeV	150 MeV	180 MeV	210 MeV
1	Front Bragg peak (-4,0)	Front Bragg peak (-10,0)	Front Bragg peak (-17,0)	Front Bragg peak (-23,0)
5	<b>Distal Bragg peak</b> (6,0)	Bragg peak (0,0)	Plateau Bragg peak (-7,0)	Plateau Bragg peak (-13,0)
9	<b>Distal Bragg peak</b> (16,0)	<b>Distal Bragg peak</b> (10,0)	<b>Distal Bragg peak</b> (3,0)	Plateau Bragg peak (-3,0)
2	<b>Lateral Bragg peak</b> (-4,11)	<b>Lateral Bragg peak</b> (-10,11)	<b>Lateral Bragg peak</b> (-17,11)	<b>Lateral Bragg peak</b> (-23,11)
6	<b>Lateral Bragg peak</b> (6,11)	<b>Lateral Bragg peak</b> (0,11)	<b>Lateral Bragg peak</b> (-7,11)	<b>Lateral Bragg peak</b> (-13,11)
10	<b>Lateral Bragg peak</b> (16,11)	<b>Lateral Bragg peak</b> al (10,11)	<b>Lateral Bragg peak</b> (3,11)	<b>Lateral Bragg peak</b> (-3,11)



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168 The material composition for PMMA and water shown in table 2 were chosen to ensure identical  
169 material composition and densities between codes. Densities were considered for room  
170 temperature.

171 **Table 2.** Material densities and compositions used for MC calculations

Material	Density (g/cm <sup>3</sup> )	Isotope	Mass fraction
Air (dry)	0.001205	<sup>14</sup> N	0.75527
		<sup>40</sup> Ar	0.01282
		<sup>16</sup> O	0.23178
		<sup>12</sup> C	0.00012
Water	0.998	<sup>16</sup> O	0.33333
		<sup>1</sup> H	0.66666
		<sup>12</sup> C	0.59985
PMMA	1.18	<sup>16</sup> O	0.31962
		<sup>1</sup> H	0.08054

172 **Monte Carlo codes and nuclear models**

173 Each participant, using a specific Monte Carlo code (1 for GEANT4, 4 for MCNPX and 1 for FLUKA),  
174 created dedicated input files for modeling the neutron energy spectra in the different positions in  
175 the water phantom. We agreed statistical uncertainties in the bins should be below 5% while for the  
176 fluence, dose calculations and calibration factors statistical uncertainties had to remain within 3%.

177 **GEANT4**

178 The binary intra-nuclear cascade model (BIC) [41] was used by setting the standard physics lists  
179 QGSP\_BIC\_HP. Furthermore, the physics list was modified with the electromagnetic physics option 3  
180 and extended for the treatment of thermal neutrons with the G4ThermalNeutronScattering physics.  
181 In order to use the thermal scattering physics for hydrogen in water, it was necessary to use  
182 TS\_H\_of\_Water defined in G4ThermalNeutronScatteringNames.cc. For all simulations GEANT4  
183 version 10.1.2 was used and neutron energy spectra were simulated.

184 **MCNPX**

185 The Monte Carlo N-Particle eXtended (MCNPX) transport code version 2.7.0 [42] was used in this  
186 exercise by 4 different institutes allowing a comparison between the MC output for the same code

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4 187 as implemented by the 4 different groups. The Los Alamos LA150H and LA150N cross section data  
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6 188 libraries were used respectively for protons and neutrons [43, 44]. Only for Carbon and Argon model  
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8 189 were used for protons due to the missing data tables. Furthermore cross section data libraries are  
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10 190 evaluated for about 40 target isotopes and for incident proton energies ranging from 1 MeV to 150  
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12 191 MeV and neutrons from 20 MeV to 150 MeV [45]. Below 20 MeV neutrons and 1 MeV protons  
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14 192 endf/b-vii.0 was used. When reaction cross section libraries are not available (> 150MeV), the Bertini  
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16 193 intra-nuclear cascade (INC) model [46] and the Dresner evaporation-fission model [47] were used as  
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18 194 default. In addition to the default Bertini- Dresner model, different combinations of Bertini and Isabel  
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20 195 [48] (for INC modeling) together with Dresner and Abla models (for evaporation phase) were  
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22 196 considered. Namely, neutron spectra were simulated for Bert-Dres, Bert-Abla, Isa-Abla and Isa-Dres  
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24 197 as well as considering the Cascade-Exciton Model (CEM version 03), combining essential features of  
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26 198 the excitation and INC models [49, 50]. For a proper evaluation of thermal neutrons, room temperature  
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28 199 cross section tables S(a,b) in water (lwtr.10t) were included based on ENDF/B-VII.0 [10].

## 29 200 FLUKA

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32 201 Physics in FLUKA is unique and unchangeable regardless of chosen settings influencing only code  
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34 202 efficiency and calculation precision [51]. For this study, the 2011.2. FLUKA version was used and the  
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36 203 HADROTherapy default settings were applied. This implicates particle transport threshold at 100 keV  
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38 204 except for neutrons simulated down to thermal energies [52]. The PEANUT package is incorporated  
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40 205 for hadron inelastic nuclear interactions [53] and modified RQMD (Relativistic Quantum Molecular  
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42 206 Dynamic) model [54] is employed for nucleus-nucleus interactions between 0.125 and 5 GeV, while  
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44 207 below 125 MeV Boltzmann Master Equation (BME) model is used [55].

## 46 208 **Neutron dose equivalent calculation from neutron spectra**

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48 209 The impact of modeling the neutron spectra on the simulated neutron dose equivalent quantity for  
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50 210 different MC codes and nuclear model was evaluated by using the method explained by Romero-  
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52 211 Expósito et al. [32]. Assuming the validity of the kerma approximation, the absorbed dose can be  
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54 212 approximated by kerma which, in turn, may be evaluated from neutron fluence through the kerma  
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56 213 factors  $k(E)$  for ICRU tissue found in the work of Siebert and Schuhmacher [56] for neutrons up to 20  
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58 214 MeV and in the work of Chadwick et al up to 150 MeV [44]. Applying the neutron quality factor as a  
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60 215 function of energy ( $Q(E)$ ), the neutron dose equivalent can be derived using the following equation:

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$$216 \quad H = \Phi \int_E Q(E) \cdot k(E) \cdot \frac{d\varphi_i(E)}{dE} \cdot dE \quad (1)$$

217 where  $\Phi$  is the total neutron fluence and  $\frac{d\varphi_i(E)}{dE}$ , the energy spectrum of the unit neutron fluence.

### 218 **Neutron dose equivalent measurements from CR 39 passive detectors**

219 The basis of dose equivalent evaluation relies in the same equation 1 with a small modification:

$$220 \quad H = \Phi \int_E Q(E) \cdot k(E) \cdot \frac{d\varphi(E)}{dE} \cdot dE \quad (2)$$

221 where  $\Phi$  is the total neutron fluence, and is obtained by the CR39 passive detector, and  $\frac{d\varphi(E)}{dE}$ , the  
222 energy spectrum of the unit neutron fluence.

223 As explained in Romero-Expósito et al. [32], total fluence can be evaluated from CR39 reading ( $N$ )  
224 taking into account an average response factor which in turn considers the fractions of each type of  
225 neutron in the spectrum:

$$226 \quad \Phi = \frac{N}{R_{\Phi}} = \frac{N}{p_{epi+th} \cdot R_{epi+th} + p_{fast} \cdot R_{fast} + p_{high} \cdot R_{high}} \quad (3)$$

227 being  $p_{epi+th}$ ,  $p_{fast}$ , and  $p_{high}$ , the thermal and epithermal fraction, fast fraction, and high energy  
228 fraction, respectively, and  $R_{epi+th}$ ,  $R_{fast}$  and  $R_{high}$ , the corresponding fluence responses.

229 Combination of equations 2 and 3 allows to derive the expression used for estimation of the  
230 calibration coefficient:

$$231 \quad \left(\frac{H}{N}\right) = \frac{\int_E Q(E) \cdot k(E) \cdot \frac{d\varphi_i(E)}{dE} \cdot dE}{p_{epi+th} \cdot R_{epi+th} + p_{fast} \cdot R_{fast} + p_{high} \cdot R_{high}} \quad (4)$$

## Results

### Benchmarking proton beam

As a first step, a general validation on proton beam ranges was carried out, for all the four mono-energetic beams. In Table 3 the interpolated R90 values from the depth dose distribution are shown in respect to the outer wall of the phantom. A good agreement between the codes was found with the largest differences in R90 value of 1.1 mm for the 180 MeV proton beam. This was considered sufficient for the purpose of this study.

**Table 3.** R90 values calculated with 3 different Monte Carlo codes (default settings) using 10 x 10 cm<sup>2</sup> parallel beam of mono-energetic protons.

R90 (cm)	110 MeV	150 MeV	180 MeV	210 MeV
GEANT4	8.98	15.62	21.58	28.06
MCNPX	9.01	15.62	21.51	28.07
FLUKA	8.98	15.62	21.47	28.02

### Neutron spectra of different MC codes inside the phantom

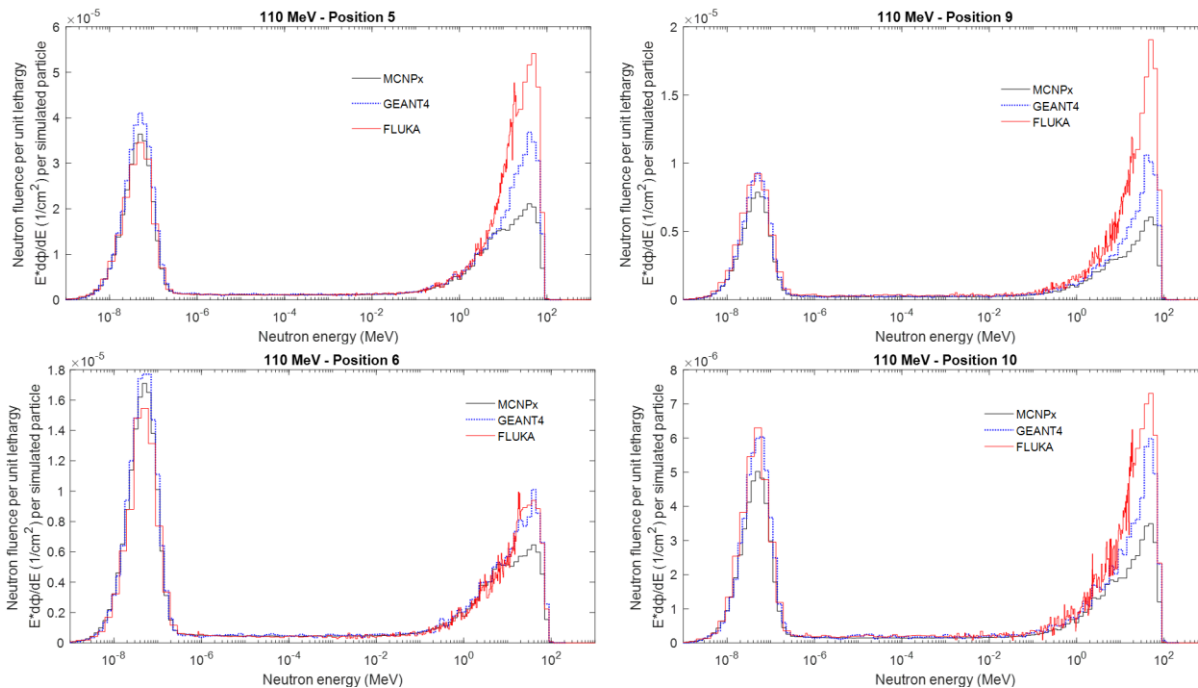
First we compare the different neutron spectra for the different codes (MCNPX, GEANT4 and FLUKA).

For MCNPX we use the default nuclear model (Bert-Dres) and we report on the data of 1 participant.

#### *110 MeV proton beam*

Figure 2 shows the results on simulated secondary neutron energy spectra inside the water phantom for 110 MeV at distal positions 5 and 9 and lateral positions 2 and 10.

Tables 4 summarizes the fluence data calculated by the different codes (default models) for 110 MeV at distal positions 5 and 9 and lateral positions 2, 6 and 10 in four neutron energy regions of thermal ( $E < 0.4$  eV), epithermal ( $0.4$  eV  $< E \leq 100$  keV), fast ( $100$  keV  $< E \leq 19.6$  MeV) and high energy ( $E > 19.6$  MeV). The thermal neutron fluences varies within 11% while for the fast and high energy neutrons, a strong energy and angular dependency is observed. In the forward scattering directions, i.e. at position 5 and 9, variations in high energy neutron fluence were found up to 46 % and 53 %, respectively, and variations on the total neutron fluence of 16% and 29%, respectively. In lateral positions 2, 6 and 10 the variation on the high energy neutron fluence was found to be lower than in



**Figure 2.** Neutron spectra simulated with different MC codes for 110 MeV proton beam at distal positions 5 and 9 and lateral positions 2 and 10 inside the water phantom.

For comparison the difference to MCNPX was calculated for GEANT4 and FLUKA (see table 4). This was done because MCNPX uses evaluated nuclear cross-sections up to 150 MeV provided in LA150H and LA150N for several materials. Moreover MCNPX has been used by 4 different participants, demonstrating very good agreement, and also particularly since we looked more explicitly into impact of MCNPX models (see section MCNPX intercomparison).

GEANT4 demonstrated a higher thermal neutron fluence compared to MCNPX for all positions except for position 2. This difference was largest for position 10 (17%). FLUKA estimations of the thermal neutron fluence was within 10% for positions 5 and 6 while an underestimation was observed for position 2 (-17%) and an overestimation for position 9 (25%) and 10 (21%). Moreover, data show that FLUKA largely overestimates the high energy neutrons in forward direction compared to MCNPX. This was 162% in position 5 and up to 200% for position 9. GEANT4 on the other hand also demonstrated an overestimation of the high energy neutron fluence which was up to 72% in position 5.

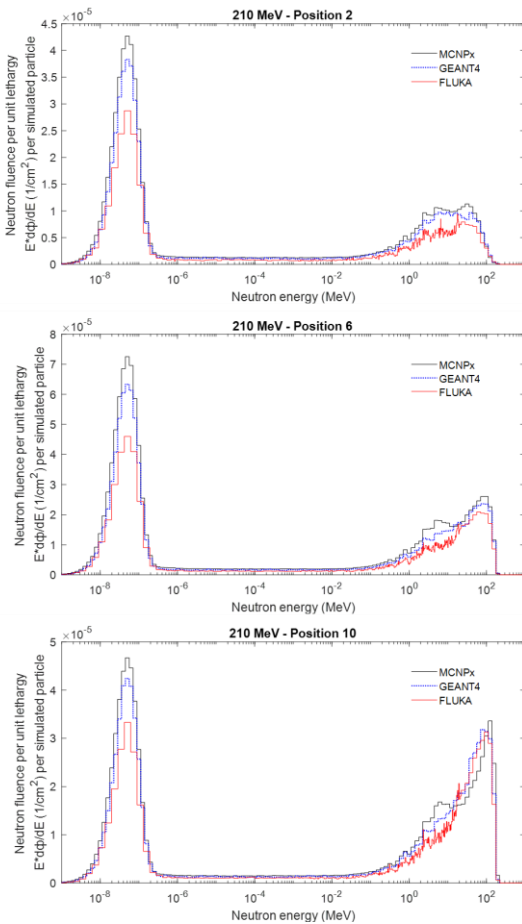
**Table 4.** Secondary neutron fluence per simulated particle in distal position 5 and 9 and lateral positions 2, 6 and 10 for 110 MeV proton beam distinguishing between Thermal ( $E \leq 0.4$  eV), Epithermal ( $0.4 \text{ eV} < E \leq 100$  keV), Fast ( $100 \text{ keV} < E \leq 19.6$  MeV) and High energy neutrons ( $E > 19.6$  MeV).

		MCNPX		GEANT4		FLUKA		Variation between codes (%)
		Bert-Dres	BIC	Difference to MCNPX	HADROTHER	Difference to MCNPX		
Position 5	Thermal	6.96E-05	7.64E-05	10%	6.84E-05	-2%	6%	
	Epith	1.46E-05	1.56E-05	6%	1.51E-05	3%	3%	
	Fast	4.42E-05	5.15E-05	17%	6.48E-05	47%	20%	
	High	2.39E-05	4.11E-05	72%	6.27E-05	162%	46%	
	TOTAL	1.52E-04	1.85E-04	21%	2.11E-04	38%	16%	
Position 9	Thermal	1.50E-05	1.71E-05	13%	1.88E-05	25%	11%	
	Epith	3.07E-06	3.43E-06	12%	4.28E-06	39%	17%	
	Fast	9.16E-06	1.14E-05	24%	1.65E-05	80%	30%	
	High	6.74E-06	1.15E-05	70%	2.02E-05	200%	53%	
	TOTAL	3.40E-05	4.34E-05	28%	5.98E-05	76%	29%	
Position 2	Thermal	4.39E-05	4.30E-05	-2%	3.64E-05	-17%	10%	
	Epith	1.03E-05	9.60E-06	-7%	7.29E-06	-29%	17%	
	Fast	2.30E-05	2.10E-05	-9%	1.49E-05	-35%	22%	
	High	4.09E-06	4.82E-06	18%	3.82E-06	-7%	12%	
	TOTAL	8.13E-05	7.84E-05	-4%	6.24E-05	-23%	14%	
Position 6	Thermal	3.26E-05	3.41E-05	5%	2.99E-05	-8%	7%	
	Epith	5.98E-06	6.33E-06	6%	5.52E-06	-8%	7%	
	Fast	1.58E-05	1.77E-05	12%	1.60E-05	2%	6%	
	High	7.02E-06	1.01E-05	44%	1.09E-05	55%	22%	
	TOTAL	6.14E-05	6.82E-05	11%	6.24E-05	2%	6%	
Position 10	Thermal	9.59E-06	1.12E-05	17%	1.16E-05	21%	10%	
	Epith	1.95E-06	2.31E-06	19%	2.54E-06	31%	13%	
	Fast	5.70E-06	7.20E-06	26%	8.70E-06	53%	21%	
	High	3.84E-06	6.21E-06	62%	8.30E-06	116%	36%	
	TOTAL	2.11E-05	2.69E-05	28%	3.12E-05	48%	19%	

*210 MeV proton beam*

Figure 3 shows the neutron spectra in lateral positions 2, 6 and 10 of a 210 MeV proton beam, as calculated by the different codes (default models). Table 5 demonstrates an average variation between codes of around 20%, which was uniform across all simulation positions. Data suggest that high energy neutron simulations showed less variation between the codes (14%, 9% and 4% for positions 2, 6 and 10, respectively) when compared to the modeling of lower energy neutrons. Moreover, simulation results at position 10 seem to have better agreement between the codes.

Looking into GEANT4 and FLUKA all these positions showed lower dose estimations when compared to MCNPX except for the high energy neutrons in position 10.



**Figure 3.** Neutron spectra simulated with different MC codes for 210 MeV proton beams at lateral positions 2, 6 and 10 inside the water phantom.

### Comparison of 110 MeV and 210 MeV proton beams

To compare data for different proton beams at a similar location, comparison of position 2 for 110 MeV (table 4 and 5) with position 10 for 210 MeV was considered (see table 5). See table 2 for relative x,y positions towards the isocenter (0,0) which is (-4,11) in position 2 for 110 MeV and (-3,11) in position 10 for 210 MeV. Both positions show similar spectral shape (figure 2 down left plot and figure 3 top plot) but the maximum neutron energy is different due to the difference in proton energy.

When comparing variations in the total fluence, these were found to be very similar and limited to 14% for 110 MeV in position 2 and 12% for 210 MeV in position 10.

In both energies and respective positions, GEANT4 shows lower values than MCNPX for low-energy neutrons and higher values for the high-energy neutrons up to 18% for 110 MeV at position 2. FLUKA tends to underestimate the neutron fluence in both cases resulting in 22 % and 23 % lower values compared to MCNPX for 110 MeV and 210 MeV, respectively, at positions 2 and 10.

**Table 5.** Secondary neutron fluence per simulated particle in lateral positions 2, 6 and 10 for 210 MeV proton beam distinguishing between Thermal ( $E \leq 0.4$  eV), Epithermal ( $0.4 \text{ eV} < E \leq 100 \text{ keV}$ ), Fast ( $100 \text{ keV} < E \leq 19.6 \text{ MeV}$ ) and High energy neutrons ( $E > 19.6 \text{ MeV}$ ).

		<u>MCNPX</u>	<u>GEANT4</u>		<u>FLUKA</u>		Variation between codes (%)
		Bert-Dres	BIC	Difference to MCNPX	HADROTHE	Difference to MCNPX	
<b>Position 2</b>	Thermal	8.18E-05	7.19E-05	-12%	5.53E-05	-32%	19%
	Epith	1.67E-05	1.46E-05	-13%	1.02E-05	-39%	24%
	Fast	3.54E-05	3.16E-05	-11%	2.12E-05	-40%	25%
	High	1.42E-05	1.27E-05	-10%	1.08E-05	-24%	14%
	TOTAL	1.48E-04	1.31E-04	-12%	9.76E-05	-34%	20%
<b>Position 6</b>	Thermal	1.38E-04	1.19E-04	-14%	9.11E-05	-34%	20%
	Epith	2.56E-05	2.15E-05	-16%	1.60E-05	-37%	23%
	Fast	5.74E-05	4.81E-05	-16%	3.52E-05	-39%	24%
	High	4.46E-05	4.13E-05	-7%	3.76E-05	-16%	9%
	TOTAL	2.66E-04	2.30E-04	-14%	1.80E-04	-32%	19%
<b>Position 10</b>	Thermal	8.92E-05	7.95E-05	-11%	6.22E-05	-30%	18%
	Epith	1.97E-05	1.71E-05	-13%	1.36E-05	-31%	18%
	Fast	5.08E-05	4.56E-05	-10%	3.58E-05	-30%	17%
	High	4.96E-05	5.38E-05	8%	5.26E-05	6%	4%
	TOTAL	2.09E-04	1.96E-04	-6%	1.64E-04	-22%	12%

### MCNPX intercomparison and evaluation of nuclear models on secondary neutron production

In this study, four different MCNPX implementations in four different institutes were used. Interestingly all participants used the same version of MCNPX 2.7. and the differences between the fluence spectra as quantified in the different energy windows was within 5% for the same nuclear model settings. Different model configurations were simulated and for proton beam energies of 110 MeV and 150 MeV variation was within 2%, which was expected because of the available cross-sections up to 150 MeV for several elements.

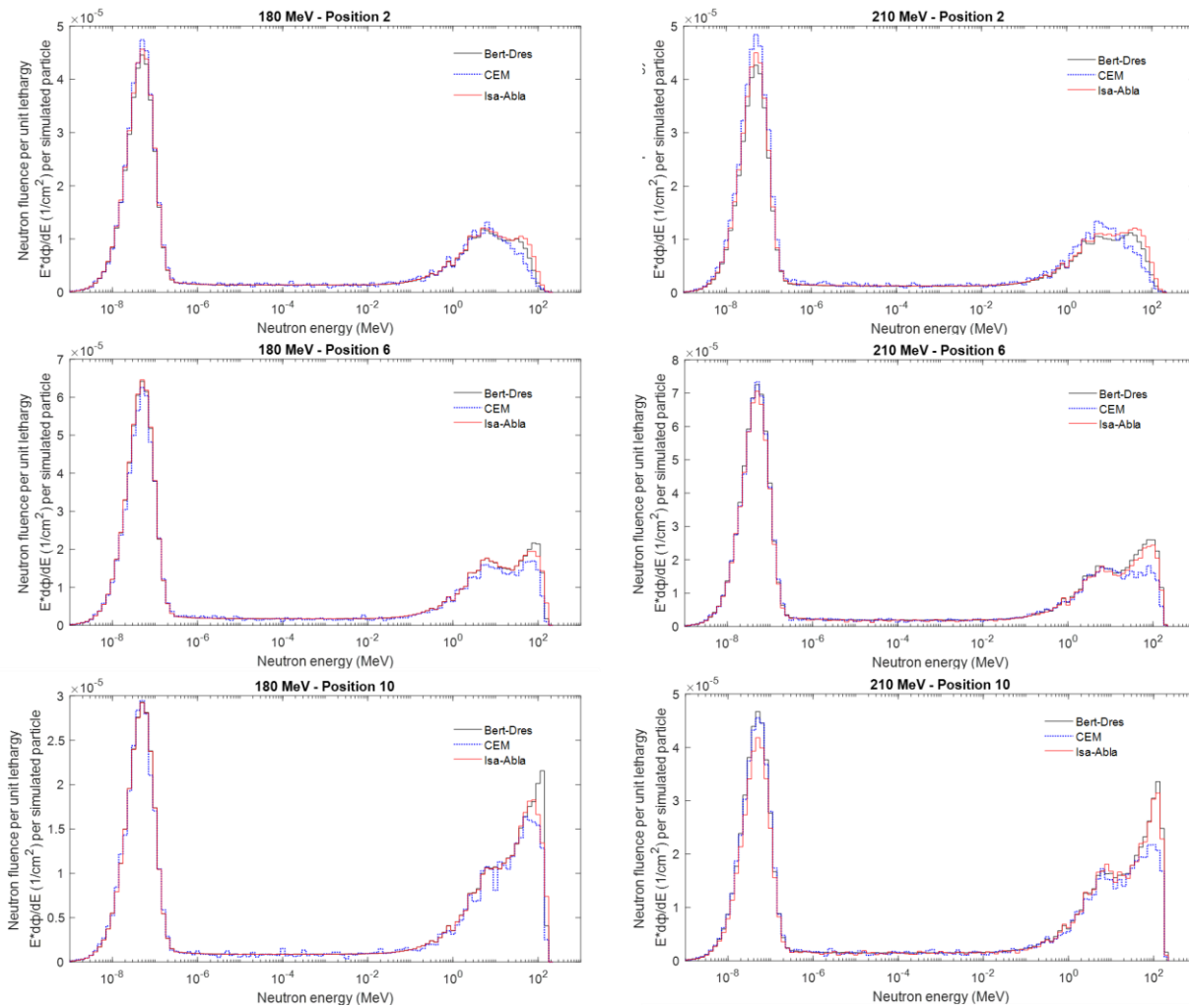


**Table 6.** Secondary neutron fluence per simulated particle for different MCNPX nuclear models in position 2, 6 and 10 for 180 and 210 MeV proton beam distinguishing between Thermal ( $E \leq 0.4$  eV), Epithermal ( $0.4$  eV  $< E \leq 100$  keV), Fast ( $100$  keV  $< E \leq 19.6$  MeV) and High energy neutrons ( $E > 19.6$  MeV).

		180MeV			Variation between models (%)	210MeV			Variation between models (%)
		Bert-Dres	CEM	Isa-Abla		Bert-Dres	CEM	Isa-Abla	
Position 2	Thermal	8.49E-05	8.84E-05	8.69E-05	2%	8.15E-05	9.27E-05	8.56E-05	7%
	Epith	1.77E-05	1.85E-05	1.82E-05	2%	1.66E-05	1.90E-05	1.75E-05	7%
	Fast	3.59E-05	3.72E-05	3.69E-05	2%	3.34E-05	3.90E-05	3.53E-05	8%
	High	1.39E-05	1.06E-05	1.65E-05	22%	1.66E-05	1.25E-05	2.00E-05	23%
	TOTAL	1.52E-04	1.55E-04	1.59E-04	2%	1.48E-04	1.63E-04	1.58E-04	5%
Position 6	Thermal	1.22E-04	1.18E-04	1.22E-04	2%	1.38E-04	1.36E-04	1.33E-04	2%
	Epith	2.29E-05	2.24E-05	2.30E-05	1%	2.55E-05	2.49E-05	2.40E-05	3%
	Fast	5.04E-05	4.71E-05	5.07E-05	4%	5.41E-05	5.34E-05	5.20E-05	2%
	High	3.66E-05	2.96E-05	3.64E-05	12%	4.85E-05	3.39E-05	4.50E-05	18%
	TOTAL	2.32E-04	2.17E-04	2.33E-04	4%	2.66E-04	2.49E-04	2.54E-04	3%
Position 10	Thermal	5.58E-05	5.58E-05	5.57E-05	0%	8.88E-05	8.84E-05	7.99E-05	6%
	Epith	1.17E-05	1.16E-05	1.16E-05	0%	1.95E-05	1.94E-05	1.87E-05	2%
	Fast	3.00E-05	2.82E-05	2.98E-05	3%	4.76E-05	4.49E-05	4.76E-05	3%
	High	3.46E-05	2.97E-05	3.30E-05	8%	5.34E-05	4.31E-05	5.16E-05	11%
	TOTAL	1.32E-04	1.25E-04	1.30E-04	3%	2.09E-04	1.96E-04	1.98E-04	4%

Table 6 and figure 4 show neutron fluences obtained with MCNPX simulations considering 3 different combinations of models Bert-Dres, CEM and Isa-Abla for primary proton energies of 180 MeV and 210 MeV at 3 different positions 2, 6 and 10. The effect on the thermal, epithermal and fast neutrons are small with variations within 8%. However, a clear difference between the three considered nuclear models is observed for the high energy neutron fluence. At position 2, the high energy neutron fluence variation between models was 22% and 23% for 180 MeV and 210 MeV protons, respectively. Position 10 shows lower variations in high energy neutron fluence for different nuclear models compared to position 2 with variation of 8% and 11% for 180 MeV and 210 MeV, respectively. In general the variation in models is higher for 210 MeV proton beams compared to 180 MeV protons, except for position 2, where a similar deviation of 22% and 23% for 180 MeV and 210 MeV, respectively, is observed (cf. figure 3 and table 6).

Comparing the three models, it is clear that Bert-Isa-Dres behaves similarly as Isa-Abla, while CEM shows a lower fluence for high energy neutrons.



**Figure 4.** Influence of MCNPX nuclear models on neutron fluence simulated at lateral positions 2 (up), 6 (middle) and 10 (down) considering proton beam energies of 180 MeV (left) and 210 MeV (right).

### Impact on calculation of stray neutron dose equivalent

Calculations of the total neutron dose equivalent (mSv/source particle) as calculated on average by the different codes are shown in table 7 together with variations in the total neutron dose equivalent computed by equation (1) and using neutron spectra of the different MC codes at different distal (5 and 9) and lateral (2, 6 and 9) positions for proton beams of 110 MeV, 150 MeV, 180 MeV and 210 MeV. In distal positions variations are generally larger compared to lateral positions and reach up to 45% at position 9 for 110 MeV protons. Obviously due to the different energy spectra and shape of the kerma and quality factors the impact on the equivalent dose (table 7) is different compared to the variation in the total fluence (see table 4 and 5). For 110 MeV we see that the variation on the

total neutron dose equivalent is larger than the variation on the total fluence which is not always observed for 210 MeV due to the lower contribution of the high energy neutrons in the spectra (see figure 2 versus figure 3).

**Table 7.** Average values of total dose equivalent from different MC codes (top) and variation on the total neutron dose equivalent calculated from spectra simulated with different codes (bottom) in distal position 5 and 9 and lateral positions 2, 6 and 10 for 110 MeV, 150 MeV, 180 MeV and 210 MeV proton beams.

<b>Average total dose equivalent [mSv per source particle]</b>				
Position	110 MeV	150 MeV	180 MeV	210 MeV
5	4.31E-11	IF	IF	IF
9	1.14E-11	4.06E-11	9.76E-11	IF
2	9.74E-12	1.40E-11	1.62E-11	1.75E-11
6	1.13E-11	2.35E-11	3.15E-11	3.73E-11
10	5.95E-12	1.68E-11	2.78E-11	4.11E-11
<b>Variation (%) on total dose equivalent between codes</b>				
Position	110 MeV	150 MeV	180 MeV	210 MeV
5	34%	IF	IF	IF
9	45%	32%	25%	IF
2	19%	24%	25%	21%
6	12%	5%	13%	15%
10	30%	16%	7%	5%

IF: in field point

In lateral positions, variations in position 2 was on average 22% for the different proton energies while variation in position 6 was generally lower on average around 11% (ranging between 5% and 15%). The largest variation for lateral positions was observed in position 10 for 110 MeV, which reached up to 30%. This can be explained by the big difference in high energy neutron region of the spectrum related to the fact that position 10 has a small angle towards 110 MeV Bragg peak (35 degrees from the field axis) and so is in a more forward direction than the other lateral positions. Using different models in MCNPX, the maximum observed relative variation for the total dose equivalent was of 5% (position 2 for 210 MeV).

### Impact on experimental evaluation of neutron dose equivalent

The impact of different MC codes and models on the calibration factor of CR39 detectors are shown in table 8 for position 6 and 10 and for different energies. Variation between models was very low and as expected for 110 MeV and 150 MeV proton energies it remained within 1%. For higher proton

energies the variation reached up to 8% for 210 MeV in position 6. Variation between codes was on average 10% and 11% for position 6 and 10, respectively.

**Table 8.** CR39 calibration factors and variation between MCNPX models and MC at lateral positions 6 and 10 for 110 MeV, 150 MeV, 180 MeV and 210 MeV proton beams.

	Proton energy	Bert-Dres	CEM	Isa-Abla	Variation models (%)	GEANT4	FLUKA	Variation codes (%)
Position 6	110 MeV	3.22E-03	3.22E-03	3.22E-03	0%	3.60E-03	3.91E-03	10%
	150 MeV	3.29E-03	3.29E-03	3.29E-03	0%	4.00E-03	4.21E-03	13%
	180 MeV	3.72E-03	3.41E-03	3.70E-03	5%	4.05E-03	4.35E-03	8%
	210 MeV	3.84E-03	3.31E-03	3.77E-03	8%	4.05E-03	4.58E-03	9%
Position 10	110 MeV	3.83E-03	3.88E-03	3.83E-03	1%	4.31E-03	4.65E-03	10%
	150 MeV	4.19E-03	4.19E-03	4.19E-03	0%	4.83E-03	5.33E-03	12%
	180 MeV	4.36E-03	4.10E-03	4.28E-03	3%	5.20E-03	5.44E-03	11%
	210 MeV	4.29E-03	3.99E-03	4.22E-03	4%	4.80E-03	5.52E-03	13%

## Discussion

This study focused on comparing three widely used MC codes, FLUKA, MCNPX and GEANT4 in the prediction of secondary neutrons spectra for the assessment of the neutron dose equivalent as well as for calibration of detectors, such as CR39. Firstly, the largest differences in calculating the neutron spectra were observed between different codes and most pronounced in the forward beam direction. Variation between the codes reached up to around 50%, with a maximum disagreement up to 200%, for the high energy neutrons in the forward positions 5 and 9 for 110 MeV. Most likely, this was related to the more prominent high energy component in the forward direction and the lack in cross section data of FLUKA and GEANT4 for neutrons above 20 MeV. MCNPX uses nuclear cross section data until 150 MeV and the present work proved that both FLUKA and GEANT4 tend to overestimate the high energy neutron fluence in forward positions up to 200% for FLUKA (110 MeV position 9) and up to 72% for GEANT4 (110 MeV position 5). For both FLUKA and GEANT4 this overestimation was mostly pronounced in distal positions (behind the Bragg peak) and to a lesser extent at lateral positions 6 and 10 which can be due to the more forwarded direction of these positions towards the Bragg peak for 110 MeV protons with respectively a 60 and 35 degrees angle from the isocenter. Indeed looking into the neutron spectra for 110 MeV proton beam it is clear that

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4 386 position 10 involves an important contribution from high energy neutrons while this is much smaller  
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6 387 at position 2.  
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8 388 In lateral positions, variations between the codes for 210 MeV are smaller and less pronounced for  
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10 389 the high energy neutrons, reaching up to 20% for the total fluence in position 10. What is noticeable  
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12 390 in these lateral positions for 210 MeV protons is that both FLUKA and GEANT4 tend to underestimate  
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14 391 the neutron fluence compared to MCNPX.  
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16 392 In general, the performance of the different codes seemed to be related to the relative position and  
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18 393 more specifically the angle towards the isocenter. In forward directions an overestimation of FLUKA  
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20 394 and GEANT4 is observed while in lateral positions (i.e. lateral position) an underestimation is present  
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22 395 (Table 3). This angular dependence is likely due to the contribution/proportion of high energy  
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24 396 neutrons prominent at forward directions. Overall the thermal neutron fluence is always most  
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26 397 pronounced for GEANT4.  
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28 398 Similarly, the total neutron dose equivalent proved to involve larger variations at distal positions  
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30 399 compared to lateral positions. Overall, increasing the proton energy decreased slightly the variation  
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32 400 between the codes which is clearly observed in position 9 and 10, respectively, going from 45% for  
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34 401 110 MeV to 25% for 180 MeV and from 30% for 110 MeV to 5% for 210 MeV. Nevertheless,  
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36 402 comparison of positions for different energies is challenging as the relative position changes towards  
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38 403 the Bragg peak and so does the spectrum and angular distribution. We did compare variation in  
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40 404 position 2 for 110 MeV with position 10 for 210 MeV, as these are positions lateral to the Bragg peak,  
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42 405 which showed comparable variations. In fact, a limitation of the study is that for the high energy  
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44 406 proton beam (210 MeV) we do not have distal positions as the beam ranged up till the end of the  
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46 407 water phantom. Nevertheless, the phantom dimensions were based on previous measurements  
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48 408 performed in EURADOS WG9 measurement campaigns [37, 40]. Moreover, in realistic clinical  
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50 409 conditions an energy of 210 MeV with the range in water exceeding 28 cm is rarely applied. In  
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52 410 addition, due to geometrical reasons, proton beam is usually not directed along the patient body so  
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54 411 the maximal neutron exposure in forward directions is limited. Therefore, most of out-of-field  
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56 412 positions will be lateral to the beam direction as studied in our work.  
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58 413 Besides the impact on the codes, the impact of the choice of the neutron models was tested in  
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60 414 MCNPX. We observed only an impact for the 180 and 210 MeV proton beams and for modeling the  
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4 415 high energy neutrons which was up to 23% for 210 MeV in position 2. Nevertheless, the impact on  
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6 416 the neutron dose equivalent was below 5% and can be considered within the statistical uncertainty  
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8 417 for the lateral positions. Interestingly the CEM model showed always lower results than the default  
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10 418 model used in MCNPX (Bertini-Dresner) and Isabel-Abla while both Bertini-Dresner and Isabel-Abla  
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12 419 show relatively good agreement. Unfortunately, these models could not be validated against  
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14 420 measurements, which was beyond the objective of the study. However, in the future EURADOS  
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16 421 Working Groups plan to organize validation experiments which could benchmark models and test  
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18 422 their performance for this specific application in proton therapy. What is noticeable though is that  
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20 423 MCNPX by default uses Bertini-Dresner, while the latest versions of MCNP6.2 uses by default the  
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22 424 CEM03 Cascade-Exciton model. Moreover, the pre-equilibrium models used by CEM03, so-called  
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24 425 “exciton” model, are more extensively developed so it could be considered as a more reliable model.  
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26 426 We did not compare the CEM03 model to FLUKA and GEANT4 data and mostly focused to compare  
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28 427 the default code setting, but clearly for high proton energies and at lateral positions, we noted overall  
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30 428 an underestimation of both FLUKA and GEANT4 towards the default MCNPX model Bertini-Dresner.  
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32 429 Finally, when using the spectra for the assessment of the calibration factor of CR39 detectors, we  
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34 430 showed the impact is within 10% for the different codes in lateral positions 6 and 10 which reached  
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36 431 up to a maximum of 13% for 150 MeV in position 6 and 210 MeV in position 10. The impact of  
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38 432 different models reached up to a maximum of 8% for 210 MeV in position 10.  
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40 433 This study describes the uncertainty associated to the MC fluence spectra to assess the calibration  
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42 434 factor and can be expected to be around 10% for lateral positions. Compared to the uncertainty  
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44 435 associated to the fluence to track density conversion from response factors of 25%, the uncertainty  
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46 436 is lower. In previous studies however the combined uncertainty, including this uncertainty with those  
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48 437 from track density and MC fluence spectra, was estimated to be around 30%. Unfortunately we were  
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50 438 not able to make a direct comparison between simulated data (mono-energetic proton beam) and  
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52 439 experimental data (Spread out Bragg peak) from the previous measurement campaign [37], but this  
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54 440 is definitely interesting and this work will be continued within EURADOS WG9.

54  
55 441 **Conclusion**

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57 442 This study demonstrated a significant impact on the neutron fluence spectra calculated by different  
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59 443 codes which has an important implication on both the calculated neutron dose equivalent and

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4 444 calibration of CR39 detectors. Use of different nuclear models in MCNPX showed less prominent  
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6 445 variations which were only visible for the high energy proton beams and modeling of high energy  
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8 446 neutrons, which results in a minor impact on the calculated neutron dose equivalent and calibration  
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10 447 of CR39.

## 11 12 448 13 14 449 **Acknowledgements**

15  
16 450 This work was carried out within EURADOS WG9 - Radiation Dosimetry in Radiotherapy. We would  
17  
18 451 like to thank our colleges for discussion about nuclear models and about existing results of neutron  
19  
20 452 dose measurements inside phantoms.

21  
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