The Influence of Energy Indexing Algorithm and Electron Substeps on MCNP4C Electron Transport: Application in Monte Carlo Simulation of X-ray Spectra in Diagnostic Radiology and Mammography

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***Abstract* — The random walk for electron transport in the MCNP4C general purpose Monte Carlo code is derived from ITS3.0, which is a well validated code for coupled electron/photon transport. The continuous slowing down approximation energy loss model is used for electron transport where the MCNP4C code breaks the electron's path into many steps. In this study, the influence of substeps and choice of electron energy indexing algorithm for electron transport on the simulation of x-ray spectra in diagnostic radiology and mammography energy range is investigated. For the simulation of x-ray spectra for tungsten (W) and molybdenum (Mo) targets at different tube voltages, the code was run in photon and electron mode with different substeps and energy indexing algorithms using default values for PHYS:P and PHYS:E cards. The simulated x-ray spectra were compared with the spectra calculated by IPEM report number 78. An average relative difference (ARD) of 11.9%, 13.7% and 14.1% were calculated between the simulated W target spectra using MCNP and ITS energy indexing algorithms at tube voltages of 80, 100 and 120 kVp, respectively. The ARD for Mo target spectra at tube voltages of 25 and 30 kVp was 16.6% and 16.7%, respectively. There is no noticeable difference between the spectra simulated using different substeps in both mammography and radiology energy range; however the simulation time increased by 43.8% and 44.2% when the substeps are set to twice the default value for W and Mo targets, respectively. Generally, there is a good agreement between the simulated and IPEM spectra, although the results suggest slight differences between the simulated spectra using different energy indexing algorithms and electron substeps which tend to be reduced by the normalization process. It is concluded that the energy indexing algorithm and electron substeps have limited influence on electron transport in MCNP4C for the purpose of simulating x-ray spectra in diagnostic radiology and mammography.**

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I. Introduction

Computer simulation of x-ray spectra is one of the most important tools for investigation of patient dose and image quality in diagnostic radiology. Since direct measurement of x-ray spectra is time consuming and remain difficult, attempts for prediction of x-ray spectra have started several decades ago. Generally the x-ray prediction models can be divided in three main categories: empirical [1] semi-empirical [2] and Monte Carlo calculations [3]. The use of the Monte Carlo method to simulate radiation transport has become one of the most accurate means of predicting the x-ray spectra even in complex geometries owing to more accurate physics modeling and incorporation of appropriate interaction cross section data. For the purpose of Monte Carlo simulation of x-ray spectrum, some groups have used self-written or in house developed computer codes [4], while others have used public domain general-purpose Monte Carlo codes such as EGS4 [5], MCNP [3] and ITS [6]. Our group has previously used the MCNP4C general-purpose Monte Carlo code running on Pentium-based PC to simulate diagnostic radiology and mammography x-ray tubes with the aim of predicting the x-ray spectra for different target/filter combinations [3]. It has been shown through comparison of simulated and measured spectra that the MCNP4C general purpose Monte Carlo code with some slight adjustment in the appropriate MCNP cards is a useful tool for generating diagnostic radiology and mammography x-ray spectra [7]. The condensed history electron transport algorithm used in MCNP4C is derived from ITS3.0, which is a well validated code for coupled electron/photon transport. The versatility of this combination, abundant literature and long term technical support and maintenance makes MCNP4C a promising code for medical physics applications [8]. The continuous slowing down approximation energy loss model is used for electron transport. To follow an electron through a significant energy loss, the MCNP4C code breaks the

electron's path into many steps. These steps are chosen to be long enough to encompass many collisions (so that multiple scattering theories are valid) but short enough so that the mean energy loss in any one step is small (so that the approximations necessary for multiple scattering theories are satisfied). According to the MCNP user manual, it is advisable to raise the number of substeps *m* per energy step if the expected number of substeps per history in a material region is less than about ten. The advantage of increasing *m* is that the angular deflection for interrupted substeps is applied to a smaller fraction of the substeps. A potential disadvantage is that the substep length may decrease to a point where the Goudsmit–Saunderson multiple scattering theory becomes less reliable. Because of the energy loss straggling, the production of bremsstrahlung and the interruption of the electron track at cell boundaries, the actual sequence of electron energies will generally deviate from the simple sequence. The precalculated transport data from a nearby energy group are therefore assigned by the so-called energy indexing algorithm. MCNP offers two energy indexing algorithms. By default, the MCNP energy indexing algorithm is applied, but the user can decide to use the ITS energy indexing algorithm instead [8].

In this study, the influence of substeps and choice of electron energy indexing algorithm for electron transport on the simulation of x-ray spectra in diagnostic radiology and mammography energy range is investigated. For simulation of x-ray spectra for tungsten and molybdenum targets at various tube voltages, the code was run in photon and electron mode with different substep sizes and energy indexing algorithms using default values for PHYS:P and PHYS:E cards to enable full electron and photon transport. The influence of voxel size was not considered on electron transport since the target size in the x-ray tube is large enough to stop all electrons without entering to the other cells.

II. Materials and Methods

A. The MCNP4C Monte Carlo Code

MCNP is a general-purpose Monte Carlo N–Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori. Important standard features that make MCNP very versatile and easy to use include a powerful general source, criticality source, and surface source; both geometry and output tally plotters; a rich collection of variance reduction techniques; a flexible tally structure; and an extensive collection of cross-section data. In order to use the code the user creates an input file that is subsequently read by MCNP. This file contains information about the problem in areas such as: the geometry specification, the description of materials and selection of cross-section evaluations, the location and characteristics of the neutron, photon, or electron source, the type of answers or tallies desired, and any variance reduction techniques used to improve efficiency.

MCNP version 4C was developed by the Monte Carlo Team in the Diagnostic Applications Group (X-5) of the Applied Physics Division (X) at Los Alamos National Laboratory. The code uses continuous-energy nuclear and atomic data libraries. Nuclear data tables in this code exist for neutron interactions, neutron-induced photons, photon interactions, neutron dosimetry or activation, and thermal particle scattering. Photon and electron data are atomic rather than nuclear in nature. Each data table available to MCNP is listed on a directory file, XSDIR. Users may select specific data tables through unique identifiers for each table, called ZAIDs. These identifiers generally contain the atomic number Z, mass number A, and library specified ID. Photon interaction tables exist for all elements from Z = 1 through Z = 94. The data in the photon interaction tables allow MCNP to account for coherent and incoherent scattering, photoelectric absorption with the possibility of fluorescent emission, and pair production. Scattering angular distributions are modified by atomic form factors and incoherent scattering functions. The electron library contains data on an element-by-element basis for atomic numbers Z=1–94. As is the case with photons, there is no distinction between isotopes for a given element. The library data contain energies for tabulation, radiative stopping power parameters, bremsstrahlung production cross sections, bremsstrahlung energy distributions, K-edge energies, Auger electron production energies, parameters for the evaluation of the Goudsmit-Saunderson theory for angular deflections based on the Riley cross section calculation, and Mott correction factors to the Rutherford cross sections also used in the Goudsmit-Saunderson theory.

To improve the efficiency of electron and photon transport, two cards (PHYS:P and PHYS:E) are implemented in MCNP for biasing some physical parameters such as production of secondary electrons by photons (IDES), coherent scattering (NOCOH), bremsstrahlung angular distribution (IBAD) and production of characteristic x-rays (XNUM). The default value for the latter (XNUM = 1) results in the analog number of tracks being sampled. If XNUM > 0, the number of photons produced is XNUM times the number that would be produced in the analog case, and a corresponding weight adjustment is made. Setting XNUM to zero turns off the production of x-ray photons by electrons.

B. Electron Substeps

To transport an electron, the MCNP4C code breaks the electron's path into many steps. These steps are chosen to be long enough to encompass many collisions (so that multiple scattering theories are valid) but short enough so that the mean energy loss in any one step is small (so that the approximations necessary for multiple scattering theories are satisfied). Except for the energy loss and straggling calculation, the detailed simulation of the electron history takes place in the sampling of the substeps. The Goudsmit-Saundeson theory is used to

sample from the distribution of angular deflections, so that the direction of the electron can change at the end of each substep. For electron transport, MCNP addresses the sampling of bremsstrahlung photons at each electron substep. The table of production probabilities is used to determine whether a bremsstrahlung photon will be created [9]. The MCNP further break the electron steps into smaller substeps. A major step of path length s is divided into m substeps, each of path length s/m. Angular deflections and the production of secondary particles are sampled at the level of these substeps. The integer m depends only on material (average atomic number Z). Appropriate values for m have been determined empirically, and range from $m = 2$ for $Z < 6$ to $m = 15$ for $Z > 91$. In some circumstances, it may be desirable to increase the value of m for a given material. In particular, a very small material region may not accommodate enough substeps for an accurate simulation of the electron's trajectory. In such cases, the user can increase the value of m with the ESTEP option on the material card. A reasonable rule of thumb is that an electron should make at least ten substeps in any material of importance to the transport problem. It should be noted that, if user set the value of m to a value smaller than the built-in default found for this material by the code, the entry is ignored [8].

C. Energy Indexing Algorithms

Because of the energy loss straggling, the production of bremsstrahlung and the interruption of the electron track at cell boundaries, the actual sequence of electron energies will generally deviate from the simple sequence. The precalculated transport data from a nearby energy group are therefore assigned by the so-called energy indexing algorithm. Although the assigned transport data will not exactly match the electron energy in each individual case, a correct average result is intended. One might say that a Monte Carlo interpolation of the transport data is performed. MCNP offers two energy indexing algorithms. By default, the so-called MCNP energy indexing algorithm is applied, but the user can decide to use the so-called ITS energy indexing algorithm instead. The MCNP energy indexing algorithm assigns the transport parameters from the energy group for which the electron energy lies in between the group boundaries. The ITS indexing algorithm, on the other hand, assigns the parameters from the group whose upper boundary is closest to the electron energy. Since the transport parameters are calculated for the upper boundary of an energy group, those assigned by the MCNP indexing algorithm correspond to an electron energy that is, on the average, located half a group too high on the energy grid. This means that a systematic error is introduced in the Monte Carlo interpolation of the transport data. The user can change the energy indexing algorithm in the MCNP code using the debug information card (DBCN). By setting the related flag (X18) in the DBCN card to zero, the MCNP energy indexing algorithm is activated while the X18=1 activate the ITS energy indexing algorithm.

D. Simulation of x-ray spectra using MCNP4C

For simulation of x-ray spectra, the code was run in photon and electron mode. The procedure starts with definition of a pencil beam electron source emitting the electrons with energy E within toward the target. We have considered a constant energy for emitted electrons. When the electrons strike the target, the code transports the electrons inside the target material until they are stopped after losing their kinetic energy. During the electrons' transport, all bremsstrahlung and characteristic x-ray production is considered. The calculated spectrum is then normalized to the total number of photons in the spectrum. The experimental set-up used in our simulation was based on the RAD 60 x-ray tube (Varian medical Systems, CA) material composition and target dimensions. We used the point detector tally measure of photon flux at a point (unit is photons/cm^2 or MeV/cm^2), which is normalized to be per starting particle. The x-ray beam is produced as electrons slow down in the anode, encounter some attenuation in the anode material depending on the anode angle and the beam direction. The x-rays propagate isotropically from the point of production, but the direction toward the *Be* window is the only one of interest for measurement of the x-ray spectra. After passing through the *Be* window, the x-ray spectrum passes through the additional filter material and air for further attenuation of the x-ray beam before the measurement point. Different energy indexing algorithms and electron substeps were considered for quantitative assessment of their effect on the simulation of x-ray spectra in both radiology and mammography energy range.

E. Reference Spectra

The generated spectra using *IPEM report No. 78* in both radiology and mammography energy ranges were used in this study as the reference spectra. The *IPEM report* contains sets of radiology and mammography x-ray spectra with much wider ranges than the previous version. This version uses XCOM photon cross section library to calculate linear attenuation coefficients of various materials. The unattenuated photon spectra are given for tungsten targets, tube potential from 30 kV to 150 kV, and target angles from 6° to 22°. The ripple value can be changed from 0 to 30%. Constant potential mammographic spectra are provided from 25 kV to 32 kV for molybdenum and rhodium targets for target angles ranging between 9° and 23°. All spectra are provided at energy bin width of 0.5 keV. These reference spectra were validated with measured spectra in a previous publication [10].

III. Results

Fig. 1a shows the simulated tungsten target spectra at 80, 100 and 120 kVp tube voltages using different energy indexing algorithms after normalization to facilitate comparison with *IPEM report No. 78*. The magnitude of produced bremsstrahlung and characteristic x-rays in the simulated

spectra with ITS energy indexing is lower than MCNP energy indexing algorithm in all energy bins. An average relative difference (ARD) of 11.9%, 13.7% and 14.1% was calculated between the *W* target simulated spectra with MCNP and ITS energy indexing algorithms at tube voltages of 80, 100 and 120 kVp, respectively. Fig. 1b shows the comparison of simulated spectra using both energy indexing algorithms without normalization. There is good agreement between simulated and reference spectra. The difference between simulated spectra with different energy indexing algorithms is reduced during the normalization process.

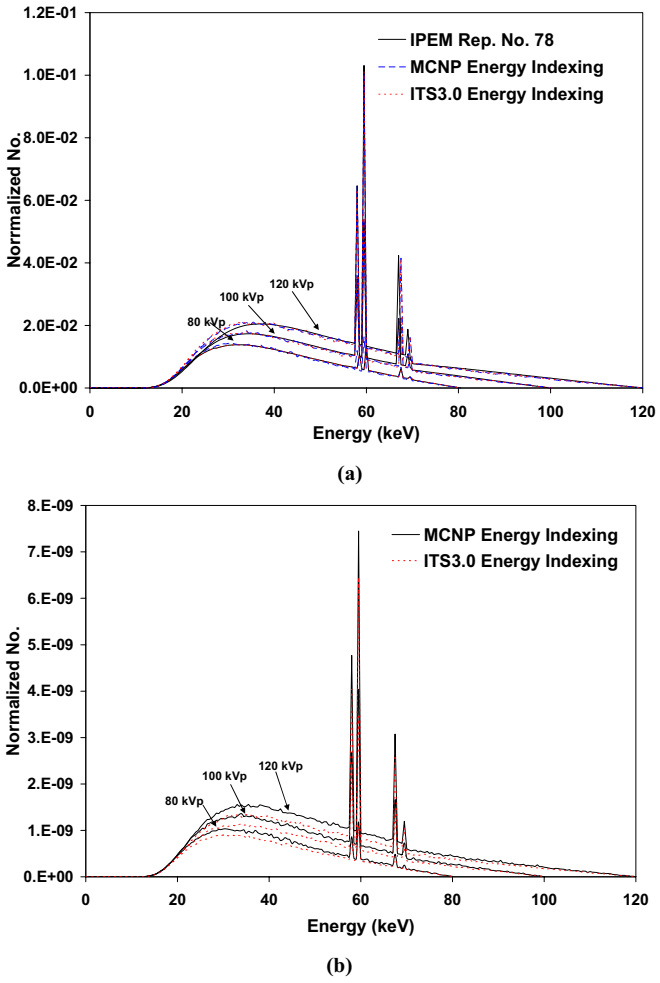


Fig. 1. Comparison of simulated spectra with IPEM report No. 78 for 12 degree *W* target and 1.5 mm Al filter at 80, 100 and 120 kVp using different energy indexing algorithms after normalization (a). Comparison of simulated spectra for 12 degree *W* target and 1.5 mm Al filter at 80, 100 and 120 kVp using different energy indexing algorithms (b). A total number of 30 million electrons were simulated. The spectra were normalized with total number of simulated electrons.

Fig. 2a and 2b show the simulated tungsten target spectra at 50 and 70 kVp and 40 and 60 kVp tube voltages using different energy indexing algorithms, respectively. The magnitude of produced bremsstrahlung x-rays in the simulated spectra with ITS energy indexing is lower than MCNP energy indexing algorithm in all energy bins.

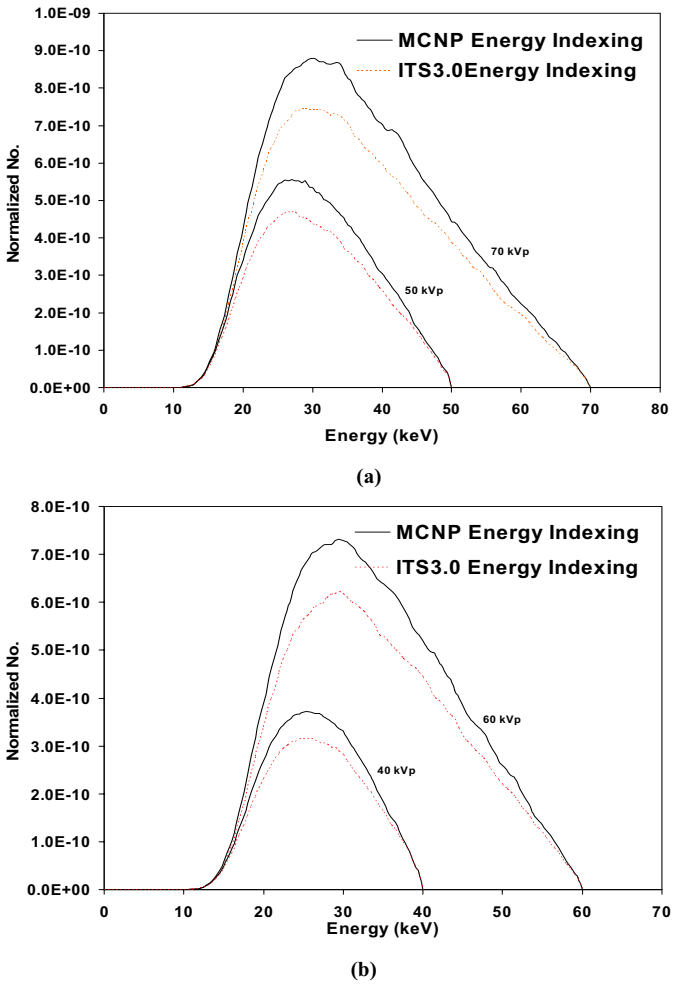


Fig. 2. Comparison of simulated spectra for 12 degree *W* target and 1.5 mm Al filter at 70 and 50 kVp using different energy indexing algorithms (a), same as above at 40 kVp and 60 kVp (b).

Fig. 3 shows the simulated molybdenum target spectra at 25 and 30 kVp tube voltages with different energy indexing algorithms. The good agreement between MCNP4C simulated spectra with IPEM for *Mo* target was already reported elsewhere [3]. Fig. 4a-b shows the simulated spectra with different numbers of electron substeps (ESTEP) for both *Mo* and *W* targets. Fig. 4c shows the impact of increasing the number of electron substeps on computation time. It was demonstrated that increasing the number of electron substeps increases the simulation time without substantial gain of accuracy for simulation of x-ray spectra (Fig. 4a-b).

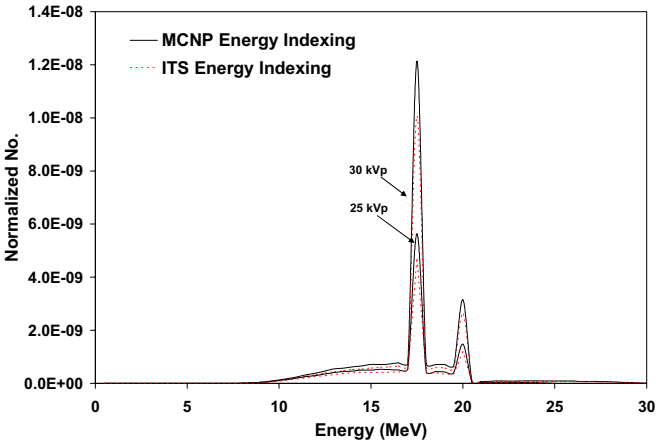
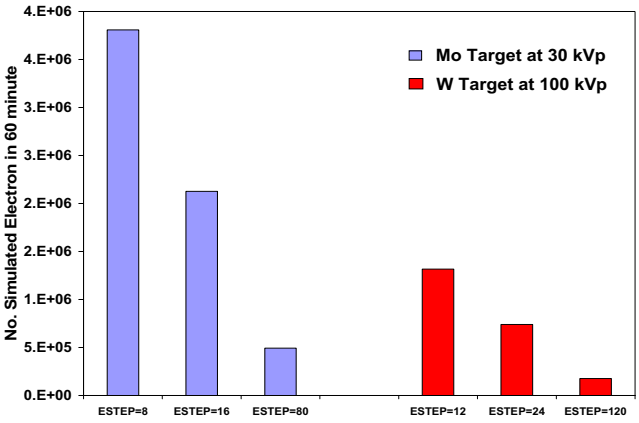
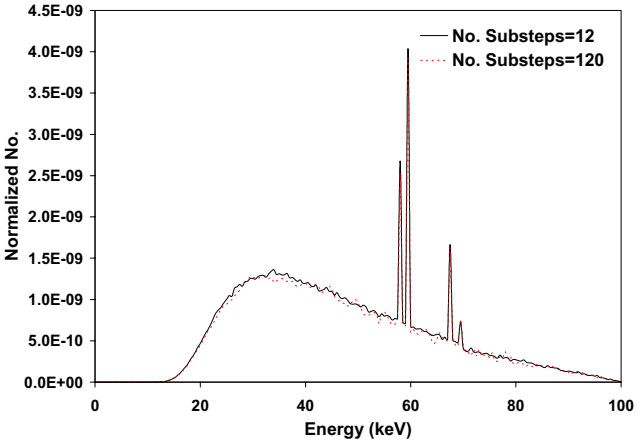


Fig. 3. Simulated spectra with 10 degree *Mo* target and 0.03 mm *Mo* filter at 25 and 30 kVp using different energy indexing algorithms.

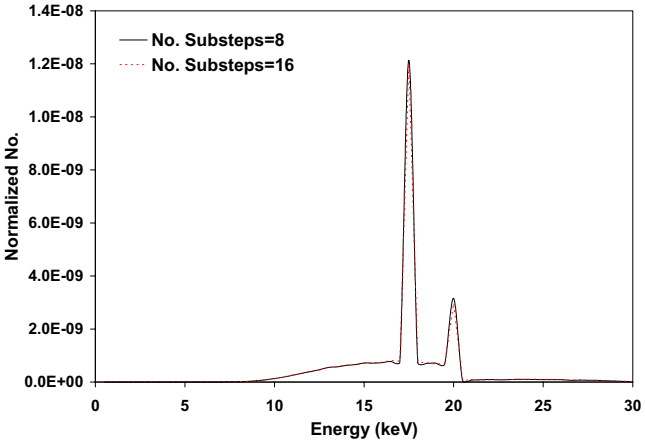


(c)

Fig. 4. Comparison of simulated spectra using various numbers of substeps in *Mo* target (a). Comparison of simulated spectra using various numbers of substeps in *W* target (b).Comparison of computation time when using different numbers of electron substeps (c).



(a)



(b)

IV. Discussion

The MCNP4C Monte Carlo code offers significant advantages for accurate simulation of x-ray spectra. More specifically, in order to improve the efficiency of electron and photon transport, two cards (PHYS:P and PHYS:E) are implemented in MCNP. The default value for the card production of characteristic x-rays (XNUM = 1) results in the analog number of tracks being sampled. There are also two adjustable parameters refereed to as electron substeps and electron energy indexing algorithm for electron transport. In this study, the influence of these two parameters on the simulation of x-ray spectra in diagnostic radiology and mammography energy range is investigated.

Although it has been reported that the energy indexing algorithm, electron substeps and voxel size have considerable influence on absorbed dose calculation [11], this study showed that these parameters are not important in modeling x-ray spectra in both radiology and mammography energy range. Figs 1-3 show that the use of the ITS energy indexing algorithm underestimates the calculated bremsstrahlung in all cases. It is obvious that increasing the electron substeps during the electron transport increases the accuracy of energy deposit calculation in the electron path length. On the other hand, increasing the number of electron substeps will definitely increase the computation time during the MC transport of electrons. This utility is important in dose calculation analysis but has not considerable effect in calculation of x-ray spectra. Fig. 4 indicates that increasing the electron substeps has not a considerable effect on the accuracy of calculated spectra but considerably increase the computation time (Fig. 4c).

V. Conclusion

Despite of the considerable impact of electron substeps and energy indexing algorithms on electron beam dosimetry calculations in radiation therapy [11], this work clearly indicates that the energy indexing algorithm and electron substeps have limited influence on MCNP4C electron transport calculations for the simulation of x-ray spectra in diagnostic radiology and mammography. To speed up the simulation process, minimum (default) values (ESTEP=8 for *Mo* and ESTEP=12 for *W*) for electron substeps are sufficient and can be recommended to end-users.

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