CALCULATION AND USE OF MULTIGROUP CROSS SECTIONS INCLUDING ELECTRON-PHOTON CASCADE FOR A 3D MONTE CARLO NEUTRON-GAMMA TRANSPORT CODE. COMPARISONS WITH MCNP-4B.

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ABSTRACT

The electron-gamma cascade is an important process which has to be taken into account in gamma ray transport calculations for radiation studies. In this work, a model originally proposed by C.M. Diop, has been implemented in the ZADIG code which calculates multigroup cross sections for any type of neutron-gamma transport code (deterministic or Monte Carlo). ZADIG can produce anisotropic group-to-group scattering matrices for gamma particles, in which electron production by gamma and bremsstrahlung production by electron are directly included. The matrices are then used in a multigroup transport code, which means that the electrons are not followed and assumed to be created and destroyed at the same point, as in the TTB (Thick Target Bremsstrahlung) option of MCNP. The matrices have been used here in the 3D Monte Carlo DIANE code, in order to make some comparisons with the code MCNP-4B. This study shows that this model for the electron-gamma cascade gives better results than the TTB option of MCNP, close to those given by a full electron transport simulation. These results can be obtained with ZADIG-DIANE in 10 minutes on a Cray T90 whereas the MCNP calculation with electrons has to be performed in parallel on 64 processors of a Cray T3E during a few hours for the same study.

1 INTRODUCTION

The electron-gamma cascade is an important process which has to be taken into account in gamma ray transport calculations for radiation studies. This phenomenom occurs when electrons, created after a photoatomic interaction, induce the production of bremsstrahlung photons during their slowing down in the matter. The bremsstrahlung may be very important, especially during the transport of high energy gamma (≈ 20 MeV). Many Monte Carlo codes, like MCNP [1], EGS4 [2] or GEANT [3], are able to simulate this process by calculating the full electron transport. However, the time execution of such a simulation is sometimes very long. This is why the default option installed in MCNP is a faster calculation using the Thick Target Bremsstrahlung (TTB) approximation. With a third model, developed by C.M. Diop at CEA/Saclay [4], the electron-gamma cascade is directly

included in a code called GAMGR which calculates multigroup cross-sections for 1D SN transport simulations. This model is used here in another CEA code, called ZADIG, which produces anisotropic group-to-group scattering matrices for any kind of neutron-gamma transport codes (deterministic or Monte Carlo). The model introduced in ZADIG is described in section 2. The calculated cross-sections have been used in a 3D Monte Carlo code called DIANE. A comparison between the results obtained with ZADIG-DIANE and those obtained with MCNP-4B is presented in section 3.

2 ELECTRON-GAMMA CASCADE MODELING

In the default TTB option of MCNP, the electrons, which are produced with a given energy and direction, are destroyed at the production point. A bremsstrahlung photon is created by sampling the production probabilities table. The electron energy is then decreased by the photon energy. This operation is repeated until the electron energy is zero. In each operation, the photon direction is obtained by sampling an angular distribution which gives the angular deflection of the photon from the initial direction of the electron. That means that the electron displacement and diffusion are neglected in this option. The C.M. Diop model, which is used in the ZADIG code only neglects the electron displacement. We will describe the three steps of the calculation (electron transport, bremsstrahlung source and multigroup assembly) and the different parameters.

2.1 ELECTRON TRANSPORT

The electron transport is divided in many slabs, in which the electron travels a length t_j and undergoes a great number of collisions (see figure 1). The electron enters into the first slab with the kinetic energy T and leaves the i^{th} slab with the kinetic energy T_i and the direction $\vec{\Omega}_e$.

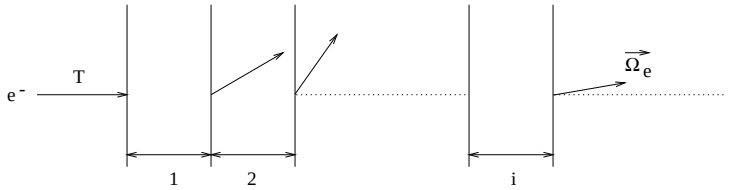

Figure 1: Electron trajectory divided in slabs

The angular distribution at the exit of each slab is calculated thanks to the multiple scattering theory of Goudsmit and Saunderson [5]. The cumulative calculation from the slab 1 to i gives the distribution :

$$g_i(\mu_e) = \frac{1}{2\pi} \sum_{l=0}^{L} \left(\frac{2l+1}{2} \right) P_l(\mu_e) \exp \left[- \sum_{j=1}^{i} Q_l(t_j, T_j) \right] \tag{1}$$

with

$$Q_l(t_j, T_j) = n t_j \int_{-1}^{+1} \sigma_D(\mu, T_j)[1 - P_l(\mu)] d\mu \tag{2}$$

where μ_e is the cosine of the angular deflection of the electron from its initial direction in the first slab, P_l the Le Gendre[1] polynomial, L its maximum order and σ_D the cross section of a single inelastic collision. With the total stopping power of the medium dT/dx, the kinetic energy T_j at the exit of the j^{th} slab is calculated as follows :

$$T_j = T - \sum_{k=1}^{j} \int_{t_k} \left(\frac{dT}{dx}\right) dx \tag{3}$$

The angular distribution $g_i(\mu_e)$ is calculated for each slab until the kinetic energy is zero.

2.2 BREMSSTRAHLUNG SOURCE

The bremsstrahlung source $S_i(T_i, k', \mu)$ produced by the electron along the i^{th} slab represents the number of photons per unit of solid angle around the $\vec{\Omega}$ direction with an energy k'. It is obtained, thanks to the angular distribution of the electron $g_i(\mu_e)$, as following :

$$S_i(T_i, k', \mu) = \int\int_{4\pi} g_i(\mu_e) n t_i \sigma_B \left(T_i, k', \vec{\Omega}.\vec{\Omega}_e\right) d\vec{\Omega}_e \tag{4}$$

where n is the medium density and σ_B is the double differential cross section of bremsstrahlung in angle and energy. The total bremstrahlung source emitted along the full electron trajectory with an initial kinetic energy T, is calculated by summing the sources of each slab.

$$P(T, k', \mu) = \sum_i S_i(T_i, k', \mu) \tag{5}$$

For the energy domain in which we are interested in ($\leq$ 20 MeV), the interactions responsible for electron or positron generation are the photoelectric effect, the incoherent Compton diffusion and the pair production. The electrons produced by photoelectric effect have a low kinetic energy and are absorbed after a very short travel. Consequently, we consider this effect as an absorption process. In ZADIG, only the Compton reaction and the pair production produce electrons or positrons which generate secondary bremsstrahlung photons. It is necessary to use the cross section of these reactions, typed r, in order to obtain the $G_r(k, k', \mu)$ transfer matrix from an initial photon with the energy k to a secondary bremsstrahlung photon with the energy k' and an angular deflection μ. This matrix is obtained after integration of the product of the electron angular distribution after a process r by the bremsstrahlung source over all the angles of electrons. For the Compton reaction the normalized matrix is calculated as follows :

$$G_{compt}(k, k', \mu) = \frac{\displaystyle\int_{-1}^{+1} \frac{d\sigma_{compt}}{d\Omega_e}(k, T, \mu_e) d\mu_e \int_0^{2\pi} P\left(T, k', \mu_\gamma^e\right) d\varphi}{\displaystyle\int_{-1}^{+1} \frac{d\sigma_{compt}}{d\Omega_e}(k, T, \mu_e) d\mu_e \int_0^{2\pi} d\varphi} \tag{6}$$

[1] The author takes the opportunity to correct here the wide-spread mistake, which consists in writing the name of the mathematician Le Gendre with a single word. Those who are surprised by this curious spelling can consult the reference [6], or a good encyclopedia and note that the famous Legendre, who was born the same year as the mathematician Le Gendre, is an important butcher who probably has nothing to do with the polynomial we are interested in.

where μ_γ^e is the cosine of the angle between the direction $\vec{\Omega}$ of the photon and the direction $\vec{\Omega}_e$ of the electron (see figure 2) :

$$\mu_\gamma^e = \cos\theta\cos\theta_e + \sin\theta\sin\theta_e\cos\varphi \tag{7}$$

For a pair production, the normalized matrix is :

$$G_{pp}^{+/-}(k,k',\mu) = \frac{\displaystyle\int_0^{k-mc^2} \frac{d\sigma_{pp}^{+/-}}{dT}(k,T)P^{+/-}(T,k',\mu)dT}{\displaystyle\int_0^{k-mc^2} \frac{d\sigma_{pp}^{+/-}}{dT}(k,T)dT} \tag{8}$$

where m is the electron mass and the symbols $+/-$ represent respectively the positron and the electron. When we do the distinction between this two particles, we write $G_{pp} = G_{pp}^{+} + G_{pp}^{-}$; otherwise $G_{pp} = 2G_{pp}^{-}$.

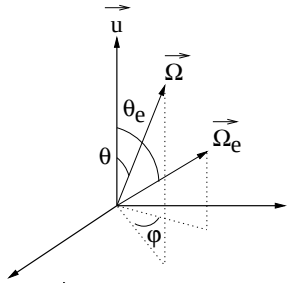

Figure 2: Calculation of $\mu_\gamma^e = \cos\left(\vec{\Omega},\vec{\Omega}_e\right)$. $\vec{u}$ = incident photon direction, $\vec{\Omega}$ = bremsstrahlung photon direction and $\vec{\Omega}_e$ = electron direction.

2.3 MULTIGROUP TRANSFER MATRIX

For a reaction r, the multigroup transfer matrix, from a group g to a group g', is obtained with the usual following calculation :

$$\sigma_{g\to g'}^r(\mu) = \frac{\displaystyle\int_g\int_{g'} \sigma_r(k)\phi(k)G_r(k,k',\mu)dkdk'}{\displaystyle\int_g \phi(k)dk} \tag{9}$$

where σ_r is the total cross section of the process and ϕ the weighting photon flux.

2.4 PARAMETERS

The input pointwise cross sections, used by the ZADIG code to produce the multigroup transfer matrices, comes from the EPDL library compiled by Livermore since 1989 [7] in the ENDF-6 format [8]. The electron-gamma cascade simulation added in ZADIG needs a few more parameters.

All the formula for the calculation of these parameters are grouped together in the reference [9].

For the electron transport, the parameters are at first the single electron diffusion cross section σ_D which gives the multiple scattering parameter Q_l. As in the GAMGR code, the parameter included in ZADIG comes from the Nigam et al. integration [10] obtained with the σ_D given by Dalitz [11]. The other important parameter for the electron transport is the total stopping power. It can come from the ICRU report [12, 13] or from the fit of this data, which is used in the GEANT code [3].

For the bremsstrahlung source, the main parameter is the cross section σ_B which is divided in two terms as following :

$$\sigma_B(T,k,\mu_\gamma^e) = \frac{d\sigma}{dk}(T,k)\frac{d\sigma}{d\Omega}(T,k,\mu_\gamma^e) \tag{10}$$

The angular differential cross section $d\sigma/d\Omega$ is the normalized σ_{2BN} of the Koch and Motz review article [14]. The energy differential cross section $d\sigma/dk$ can come from the reference [15] or from the fit of this data, used in the GEANT code [3]. The last parameter is the pair production differential cross section in electron kinetic energy. This parameter is calculated with the Bethe-Heitler formula [16] which does not distinguish between electron and positron.

3 ZADIG VALIDATION

In order to make some comparisons with the MCNP-4B code, the multigroup matrices produced by ZADIG have been used in a 3D Monte Carlo code called DIANE developed at CEA. We will first show the influence of the electron-gamma cascade on the ZADIG multigroup matrices for the lead ($Z = 82$) and then present two types of calculations (without and with bremsstrahlung) with ZADIG-DIANE and MCNP-4B. The results of these simulations are summarized on the figures 5 and 6 at the end of the section.

3.1 BREMSSTRAHLUNG INFLUENCE ON THE MULTIGROUP MATRICES

The transfer matrices have been calculated by ZADIG for 55 energy groups between 0.55 and 20.1 MeV. Even with the bremsstrahlung, all the group-to-group photon scattering matrices are calculated in less than one minute on a Cray T90. The figure 3 shows the transfer cross section from the group [4.7-5] MeV to the lower energy groups, with and without bremsstrahlung. We see on this figure that the electron-gamma cascade increases the transfer towards the lower energies. For example, the transfer to 1 MeV is increased by a factor more than two when this process is taken into account.

The same kind of transfer matrix has been calculated for the group [19.9-20.1] MeV, which is close to a 20 MeV pointwise energy. The results, presented in the figure 4, show that for this high energy, the bremsstrahlung influence is much more important. Now, the transfer to 1 MeV is increased by a factor 60. Consequently, in order to focus on the validation on the electron-gamma cascade simulation, all the photon transport calculations presented hereafter use a [19.9-20.1] MeV gamma source which maximizes the bremsstrahlung effect.

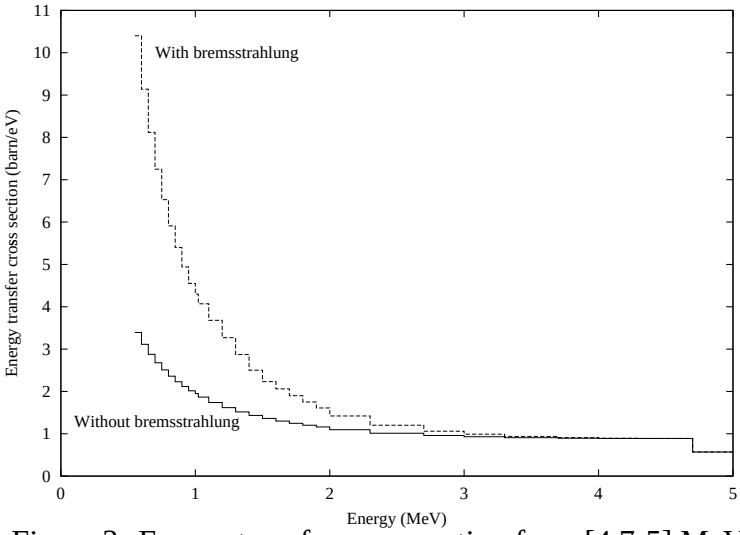

Figure 3: Energy transfer cross section from [4.7-5] MeV

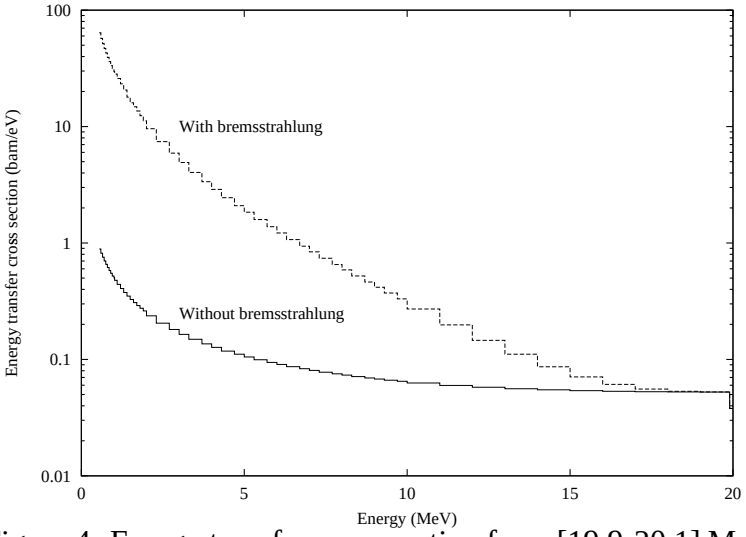

Figure 4: Energy transfer cross section from [19.9-20.1] MeV

3.2 SIMULATION WITHOUT BREMSSTRAHLUNG

A first set of calculations without bremsstrahlung have shown non negligible discrepancies between ZADIG-DIANE and MCNP. This is due to the photon interaction library. As it has been explained in section 2.4, DIANE uses the EPDL library distributed by Livermore since 1989. The mcplib02 library of MCNP is based on the same data except for photons below 10 MeV which use a much older source [17]. The main differences come from the pair production cross section. Seeing that these differences have an influence on our calculations, we have produced for this study a new mcplibcea library for MCNP, using the pair production Livermore data for all energies.

Two types of geometry are tested, a simple gamma loss calculation in a sphere and a more complex simulation of gamma transport across a plate.

Lead sphere

In this study, an isotropic source of photons with an energy of 20 MeV is launched in the center of a 10 cm radius lead sphere. The simulation gives the energy spectrum of the photons leaving the sphere, calculated on eight groups. It is important not to confuse these groups with the multigroup division for the DIANE simulation. The results obtained with MCNP and DIANE are summarized on the table I, associated with the statistical error. All the errors are given for a 95% confidence interval. The last column which gives the relative difference between the two codes shows that there is a good agreement (around 2% for the total answer) except at low energy, which is perhaps partly due to the small differences between mcplibcea and EPDL.

Table I: Comparison MCNP(libcea)-DIANE (lead sphere without brem)

group	E1	E2	MCNP	stat.(%)	DIANE	stat.(%)	Diff.(%)
1	0.55	2	1.10E-03	0.24	1.06E-03	0.28	-4.11
2	2	4	8.23E-04	0.28	7.97E-04	0.25	-3.18
3	4	6	3.52E-04	0.44	3.48E-04	0.40	-1.10
4	6	8	1.89E-04	0.60	1.89E-04	0.57	-0.19
5	8	10	1.19E-04	0.74	1.18E-04	0.75	-0.46
6	10	15	1.68E-04	0.64	1.67E-04	0.68	-0.46
7	15	19.9	9.38E-05	0.84	9.32E-05	0.97	-0.65
8	19.9	20.1	9.17E-04	0.26	9.14E-04	0.30	-0.35
Total			3.77E-03	0.14	3.69E-03	0.14	-2.13

Lead plate

In this second configuration, photons of 20 MeV are launched in a 2 degree angle cone towards a lead plate. The calculation gives the energy spectrum of the photons reaching a detector located at 1.28 m behind the plate. The distance source-plate is 3.3 m, the plate thickness is 10 cm and the detector is a $15.36 \times 15.36\ \mathrm{cm}^2$ square. The results are summarized on the table II. There is a good agreement between the two codes (less than 1% for the total answer) but one group shows a non negligible difference. However, this discrepancy which is still not explained at the moment, has almost no influence on the total result.

Table II: Comparison MCNP(libcea)-DIANE (lead plate without brem)

group	E1	E2	MCNP	stat.(%)	DIANE	stat.(%)	Diff.(%)
1	0.55	2	3.69E-06	3.30	3.58E-06	0.84	-3.00
2	2	4	3.39E-06	3.44	3.31E-06	1.04	-2.61
3	4	6	1.62E-06	4.98	1.65E-06	1.48	+2.41
4	6	8	1.01E-06	6.30	1.00E-06	2.16	-0.47
5	8	10	6.66E-07	7.74	6.75E-07	2.81	+1.30
6	10	15	4.30E-06	3.06	4.65E-06	1.06	+8.28
7	15	19.9	1.90E-05	1.44	1.89E-05	0.55	-0.92
8	19.9	20.1	2.58E-04	0.40	2.55E-04	0.00	-1.10
Total			2.91E-04	0.38	2.88E-04	0.04	-0.96

3.3 SIMULATION WITH BREMSSTRAHLUNG

The two previous configurations are now treated with bremsstrahlung. The MCNP calculations have been performed with the TTB default option and with the full electron transport. The last simulation which is the most complete is considered as a reference for all the difference calculations.

Lead sphere

The results obtained with MCNP are summarized in table III. The column *elec/norm* gives the ratio between a simulation with electron and the simulation without bremsstrahlung presented in table I. We first see that the bremsstrahlung effect is very important. The total number of photons is increased by almost a factor 20. Below 2 MeV, this factor is almost 40 because the bremsstrahlung increases the transfer towards the lower energies. The discrepancy between the TTB approximation and the full electron transport simulation is around 24% for the total result. The table IV shows the DIANE results and the relative difference with the electron transport simulation of MCNP. We see that the spectrum is similar and that the total result is around 14% lower than the MCNP one. The model seems to be acceptable and the ZADIG-DIANE calculation is much faster (10 minutes on a Cray T90) than the MCNP simulation, which has been performed in parallel on 64 processors of a Cray T3E during 45 minutes with the TTB option and almost 6 hours with the electrons.

Table III: MCNP(libcea) (lead sphere with brem)

group	E1	E2	electron	stat.(%)	elec/norm	ttb	stat.(%)	Diff(%)
1	0.55	2	4.18E-02	0.10	37.9	5.50E-02	0.06	+31.51
2	2	4	2.12E-02	0.14	25.8	2.52E-02	0.08	+18.65
3	4	6	5.72E-03	0.26	16.3	6.36E-03	0.14	+11.08
4	6	8	1.97E-03	0.46	10.4	2.06E-03	0.26	+4.86
5	8	10	7.92E-04	0.72	6.7	7.79E-04	0.42	-1.66
6	10	15	5.32E-04	0.86	3.2	4.96E-04	0.52	-6.85
7	15	19.9	1.11E-04	1.90	1.2	1.06E-04	1.12	-4.48
8	19.9	20.1	9.16E-04	0.66	1.0	9.17E-04	0.38	-0.04
Total			7.30E-02	0.08	19.4	9.09E-02	0.04	+24.37

Table IV: ZADIG-DIANE (lead sphere with brem)

group	E1	E2	loss	stat.(%)	brem/norm	Diff (%)
1	0.55	2	3.55E-02	0.15	33.5	-15.02
2	2	4	1.83E-02	0.15	23.0	-13.57
3	4	6	4.94E-03	0.30	14.2	-13.67
4	6	8	1.67E-03	0.51	8.8	-15.28
5	8	10	6.27E-04	0.80	5.3	-20.79
6	10	15	4.15E-04	0.90	2.5	-21.99
7	15	19.9	9.82E-05	1.57	1.1	-11.27
8	19.9	20.1	9.18E-04	0.50	1.0	+0.15
Total			6.25E-02	0.10	17.0	-14.42

Lead plate

The results obtained with MCNP are summarized in table V. This time, the last column shows the ratio between the calculation results with TTB and with electrons. The TTB simulation gives an aberrant result more than ten times larger than the full electron transport result. This ratio is even around 15 for low energies. This is due to the fact that the TTB approximation neglects all the electron diffusion processes. Therefore a lot of bremsstrahlung photons travel towards the detector in the simulation, whereas in reality photons are much more scattered and a large fraction should not reach the detector. This is why the electron simulation shows that the bremsstrahlung effect is less important than in the sphere calculation. Nevertheless, the ratio *elec/norm* is greater than three and the number of low energies photons reaching the detector, which is very low, is 70 times greater with bremsstrahlung.

Table V: MCNP(libcea) (Lead plate with brem)

group	E1	E2	electron	stat.(%)	elec/norm	ttb	stat.(%)	ttb/elec
1	0.55	2	2.66E-04	1.22	72.0	4.03E-03	0.34	15.1
2	2	4	2.49E-04	1.26	73.3	3.85E-03	0.32	15.5
3	4	6	9.69E-05	2.04	60.0	1.26E-03	0.56	13.0
4	6	8	4.30E-05	3.04	42.8	4.41E-04	0.96	10.2
5	8	10	2.11E-05	4.34	31.7	1.63E-04	1.56	7.7
6	10	15	1.79E-05	4.72	4.2	8.87E-05	2.12	5.0
7	15	19.9	2.02E-05	4.44	1.1	2.27E-05	4.20	1.1
8	19.9	20.1	2.57E-04	1.24	1.0	2.57E-04	1.24	1.0
Total			9.72E-04	0.64	3.3	1.01E-02	0.22	10.4

The ZADIG-DIANE results are presented on table VI. We clearly see that the modeling installed in ZADIG is better than the TTB option. With the CEA code, which takes into account the electron diffusion distribution, the total number of photons is less than 17% lower than the result given by the complete electron simulation of MCNP. Nevertheless, the agreement is not perfect and there is some non negligible differences for a few groups, even if the very low number of photons in these groups has almost no influence on the total result. The ZADIG-DIANE computing time is still very low (10 minutes on a T90), to be compared to more than five hours on 64 processors of a T3E for MCNP with electrons.

Table VI: ZADIG-DIANE (Lead plate with brem)

group	E1	E2	detector	stat.(%)	brem/norm	Differ (%)
1	0.55	2	2.17E-04	0.69	60.5	-18.47
2	2	4	1.92E-04	0.89	58.2	-22.68
3	4	6	7.08E-05	0.92	42.8	-26.93
4	6	8	2.92E-05	1.03	29.2	-32.06
5	8	10	1.29E-05	1.20	19.1	-39.03
6	10	15	1.31E-05	1.73	2.8	-26.87
7	15	19.9	1.89E-05	1.94	1.0	-6.55
8	19.9	20.1	2.55E-04	0.10	1.0	-0.99
Total			8.09E-04	0.30	2.8	-16.72

The various energy spectra presented in this section are summarized in the figure 5 for the sphere and the figure 6 for the plate. These curves show the ratio $n_i/\Delta E_i$ function of the energy, where n_i is the photon number in the group i and ΔE_i the difference between the energy boundaries.

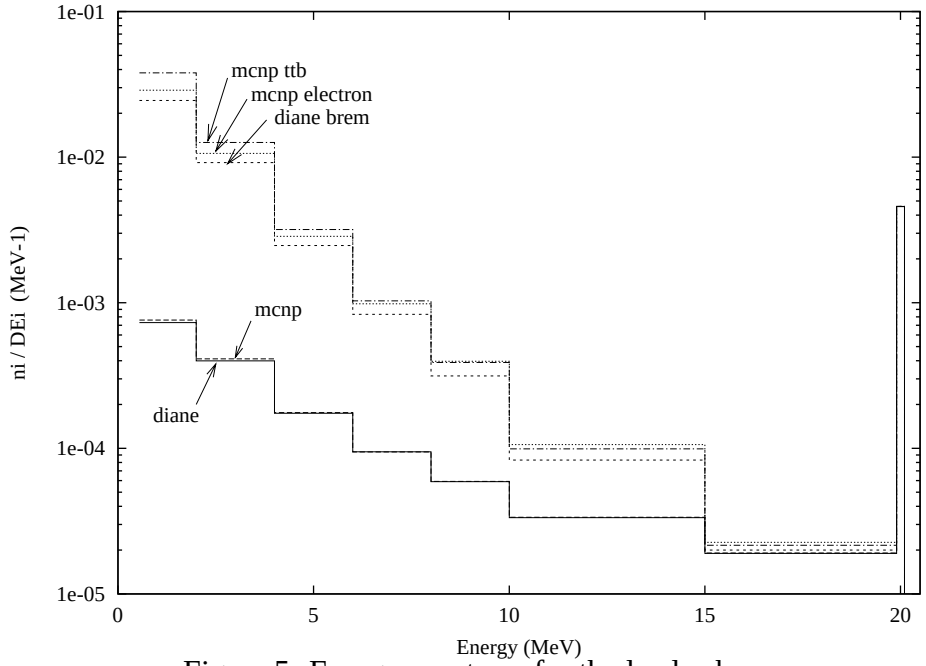

Figure 5: Energy spectrum for the lead sphere

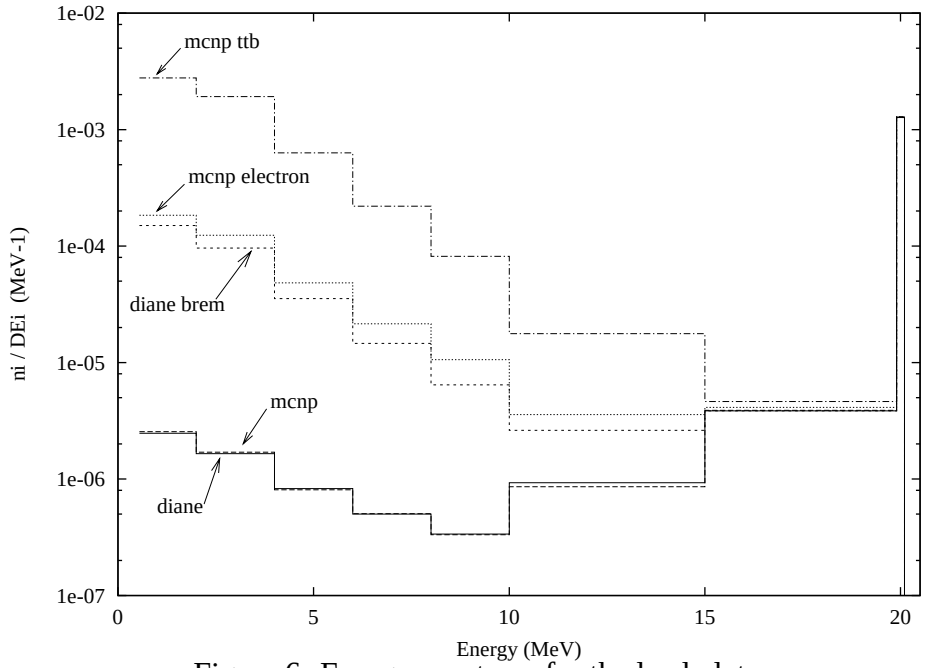

Figure 6: Energy spectrum for the lead plate

4 CONCLUSION

The model of the electron-gamma cascade, originally proposed by C.M. Diop, has been implemented in the CEA ZADIG code, which calculates multigroup cross sections for any type of neutron-gamma transport code (deterministic or Monte Carlo). These constants have been used here in the 3D Monte Carlo DIANE code in order to perform some comparisons with MCNP-4B. Two important conclusions may be drawn from these calculations. First, the TTB approximation installed by default in MCNP can give aberrant results because the electron diffusion process is neglected. Secondly, the model implemented in ZADIG, which takes into account this process, gives better results close to those given by a full electron transport simulation of MCNP. These results can be obtained with ZADIG-DIANE in 10 minutes on a Cray T90 whereas the MCNP calculation with electrons has to be performed in parallel on 64 processors of a Cray T3E during a few hours for the same study.

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