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IMPORTANCE ITERATION IN MORSE MONTE CARLO CALCULATIONS

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IMPORTANCE ITERATION IN MORSE MONTE CARLO CALCULATIONS

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Abstract-*An expression to calculate point values (the expected detector response of a particle emerging from a collision or the source) is derived and implemented in the MORSE-SGC/S Monte Carlo code. It is outlined how these point values can be smoothed as a function of energy and as a function of the optical thickness between the detector and the source. The smoothed point values are subsequently used to calculate the biasing parameters of the Monte Carlo runs to follow.*
The method is illustrated by an example, which shows that the obtained biasing parameters lead to a more efficient Monte Carlo calculation.

1 Introduction

To enhance the efficiency of Monte Carlo calculations, biasing schemes are used to modify probability density functions (PDF) in Monte Carlo codes, such that important parts of the geometry and energy range are more often sampled, while other parts are scarcely sampled. A biasing scheme which makes use of importance functions is generally called importance sampling or importance biasing. It is well known that properly chosen importance functions can lead to zero variance schemes for last event estimators [1] and collision estimators if the particle is not allowed to terminate [2]. Although such zero variance schemes are highly theoretical because knowledge of the final solution is required in advance of the Monte Carlo calculation, approximations to the optimum importance functions are likely to reduce the variance in Monte Carlo calculations.

Optimum importance sampling requires knowledge of both the event value, the expected detector response of a particle entering a collision, and the point value, the expected detector response of a particle emerging from a collision or the source. Calculating these value functions exactly and performing a Monte Carlo calculation with biased PDFs is generally less efficient than an unbiased Monte Carlo calculation only. An often employed calculation scheme, therefore, is to calculate point values by use of a one- or two-dimensional discrete ordinates code in an approximate geometry or by use of an approximate calculational method in an exact geometry. If the proper source function is used, the point value is equal to the "adjoint flux" in the output of such a code, and this point value can be used to calculate input biasing parameters for the subsequent Monte Carlo calculation.

For some geometries, the above mentioned methods to get insight into the value functions of the problem under consideration fail, because of geometrical difficulties like voids and ducts. In case of complex three-dimensional geometries, one- or two-dimensional discrete ordinates codes cannot even be used to get approximate answers to the value functions and other approximate methods or physical insight must be used to bias Monte Carlo calculations properly. One method is to estimate volume averaged value functions in the forward Monte Carlo run itself. These point values can then be used as a biasing function in the next Monte Carlo run to enhance the efficiency of that run. Booth defined point values in the MCNP Monte Carlo code as the ratio of the total score due to particles and their progenies leaving a cell, and the total weight leaving the cell [3] (or the same definition with particles entering a cell [4]).

In this article a similar definition (but not exactly the same) of point values averaged over geometrical zones, energy groups, and the angular space 4π is used to calculate biasing parameters and weight window limits for Monte Carlo calculations with the MORSE-SGC/S code [5]. The theory of importance biasing in Monte Carlo calculations is given in Section 2 and the implementation of the theory in the MORSE Monte Carlo code in Section 3. Section 4 describes a method to calculate point values and event values averaged over volume, energy and angular space in a forward Monte Carlo run by the MORSE code. In this section, emphasis will be put to the point value because in shielding calculations with a non-absorption probability of nearly unity, the difference between the point value and the event value is very small, as will be shown in that Section. The way to calculate biasing parameters from point values is given in literature [6] and is shortly outlined in Section 5. Finally, an example which illustrates the method is given in Section 6.

2 Importance Biasing in Monte Carlo Calculations

The integral transport equation for the emergent particle density $\chi(\boldsymbol{r}, E, \boldsymbol{\Omega})$ reads [7]:

$$\chi(\boldsymbol{r}, E, \boldsymbol{\Omega}) = S(\boldsymbol{r}, E, \boldsymbol{\Omega}) + \int_{allV} \int_{4\pi} \int_{0}^{\infty} \chi(\boldsymbol{r}', E', \boldsymbol{\Omega}') L(\boldsymbol{r}' \rightarrow \boldsymbol{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) dE' d\Omega' dV' =$$

$$S(\boldsymbol{r}, E, \boldsymbol{\Omega}) + \int_{allV} \int_{4\pi} \int_{0}^{\infty} \chi(\boldsymbol{r}', E', \boldsymbol{\Omega}') T(\boldsymbol{r}' \rightarrow \boldsymbol{r}, E', \boldsymbol{\Omega}') C(\boldsymbol{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) dE' d\Omega' dV' \quad (1)$$

where $S(\boldsymbol{r}, E, \boldsymbol{\Omega})$ is the source density, $T(\boldsymbol{r}' \rightarrow \boldsymbol{r}, E', \boldsymbol{\Omega}')$ the transport kernel, which is the probability that a particle emerging from a collision or the source at $\boldsymbol{r}'$ with energy E' and direction $\boldsymbol{\Omega}'$ enters its next collision in a unit volume around $\boldsymbol{r}$, and $C(\boldsymbol{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega})$ is the collision kernel. $C(\boldsymbol{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) dE d\Omega$ describes the probability that a particle entering a collision at $\boldsymbol{r}$ scatters from energy E' to dE around E and from direction $\boldsymbol{\Omega}'$ to solid angle $d\Omega$ around $\boldsymbol{\Omega}$. The total transport kernel L is defined as:

$$L(\boldsymbol{r}' \rightarrow \boldsymbol{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) = T(\boldsymbol{r}' \rightarrow \boldsymbol{r}, E', \boldsymbol{\Omega}') C(\boldsymbol{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) \quad (2)$$

Instead of describing the transport process in terms of the emergent particle density, a description in terms of the collision density could also be used. This gives:

$$\psi(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \int_{allV} S(\boldsymbol{r}', E, \boldsymbol{\Omega}) T(\boldsymbol{r}' \rightarrow \boldsymbol{r}, E, \boldsymbol{\Omega}) dV' +$$

$$\int_{allV} \int_{4\pi} \int_{0}^{\infty} \psi(\boldsymbol{r}', E', \boldsymbol{\Omega}') C(\boldsymbol{r}', E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) T(\boldsymbol{r}' \rightarrow \boldsymbol{r}, E, \boldsymbol{\Omega}) dE' d\Omega' dV' \quad (3)$$

Eqs. (1) and (3) are equivalent in the sense that they describe the same transport process. Because a Monte Carlo calculation consists of repeatedly calls of the transport kernel and the collision kernel, both the emergent particle density and the collision density are calculated.

The point value function is described by an equation mathematically adjoint to Eq. (1):

$$\chi^*(\boldsymbol{r}, E, \boldsymbol{\Omega}) = h(\boldsymbol{r}, E, \boldsymbol{\Omega}) +$$

$$\int_{allV} \int_{4\pi} \int_{0}^{\infty} \chi^*(\boldsymbol{r}', E', \boldsymbol{\Omega}') T(\boldsymbol{r} \rightarrow \boldsymbol{r}', E, \boldsymbol{\Omega}) C(\boldsymbol{r}', E \rightarrow E', \boldsymbol{\Omega} \rightarrow \boldsymbol{\Omega}') dE' d\Omega' dV' \quad (4)$$

where $h(\boldsymbol{r}, E, \boldsymbol{\Omega})$ is the detector response function for the emergent particle density. With this source function the point value $\chi^*(\boldsymbol{r}, E, \boldsymbol{\Omega})$ has the meaning of the expected detector response of particles emerging from the source or a collision at $(\boldsymbol{r}, E, \boldsymbol{\Omega})$, as will be shown later on.

The event value function, which has the meaning of the expected detector response of particles entering a collision, can be described by an equation adjoint to Eq. (3):

$$\psi^*(\boldsymbol{r}, E, \boldsymbol{\Omega}) = g(\boldsymbol{r}, E, \boldsymbol{\Omega}) +$$

$$\int_{allV}\int_{4\pi}\int_{0}^{\infty}\psi^*(\boldsymbol{r}',E',\boldsymbol{\Omega}')C(\boldsymbol{r},E\rightarrow E',\boldsymbol{\Omega}\rightarrow\boldsymbol{\Omega}')T(\boldsymbol{r}\rightarrow\boldsymbol{r}',E',\boldsymbol{\Omega}')dE'd\boldsymbol{\Omega}'dV' \tag{5}$$

where $g(\boldsymbol{r},E,\boldsymbol{\Omega})$ is the detector response function for the collision density.

It will now be shown that the point value has indeed the meaning of the expected detector response of a particle emerging from a collision or the source. Multiplying Eq. (1) with the point value $\chi^*(\boldsymbol{r},E,\boldsymbol{\Omega})$ and Eq. (4) with the emergent particle density $\chi(\boldsymbol{r},E,\boldsymbol{\Omega})$, integrating both resultant equations over whole phase space and subtracting one equation from the other, leads to the following expression for the total detector response D:

$$D=\int_{allV}\int_{4\pi}\int_{0}^{\infty}h(\boldsymbol{r},E,\boldsymbol{\Omega})\chi(\boldsymbol{r},E,\boldsymbol{\Omega})dEd\boldsymbol{\Omega}dV=\int_{allV}\int_{4\pi}\int_{0}^{\infty}S(\boldsymbol{r},E,\boldsymbol{\Omega})\chi^*(\boldsymbol{r},E,\boldsymbol{\Omega})dEd\boldsymbol{\Omega}dV \tag{6}$$

Likewise it can be shown that the event value has the meaning of the expected detector response of a particle entering a collision.

The detector response function of the emergent particle density is related to the detector response function of the collision density via:

$$h(\boldsymbol{r},E,\boldsymbol{\Omega})=\int_{allV}T(\boldsymbol{r}\rightarrow\boldsymbol{r}',E,\boldsymbol{\Omega})g(\boldsymbol{r}',E,\boldsymbol{\Omega})dV' \tag{7}$$

Likewise the two value functions are related to each other. From Eqs. (4) and (5) it is clear that $\chi^*(\boldsymbol{r},E,\boldsymbol{\Omega})$ is related to $\psi^*(\boldsymbol{r}',E,\boldsymbol{\Omega})$ via:

$$\chi^*(\boldsymbol{r},E,\boldsymbol{\Omega})=\int_{allV}\psi^*(\boldsymbol{r}',E,\boldsymbol{\Omega})T(\boldsymbol{r}\rightarrow\boldsymbol{r}',E,\boldsymbol{\Omega})dV' \tag{8}$$

and that $\psi^*(\boldsymbol{r},E,\boldsymbol{\Omega})$ can be described in terms of $\chi^*(\boldsymbol{r},E',\boldsymbol{\Omega}')$ via:

$$\psi^*(\boldsymbol{r},E,\boldsymbol{\Omega})=g(\boldsymbol{r},E,\boldsymbol{\Omega})+\int_{4\pi}\int_{0}^{\infty}\chi^*(\boldsymbol{r},E',\boldsymbol{\Omega}')C(\boldsymbol{r},E\rightarrow E',\boldsymbol{\Omega}\rightarrow\boldsymbol{\Omega}')dE'd\boldsymbol{\Omega}' \tag{9}$$

In Monte Carlo calculations, the transport kernel and the collision kernel are repeatedly called to track the particles through phase space until they are absorbed. A modified stochastic process can be defined, which does not describe the transport of particles itself, but of "expected detector responses" of particles. The density of such an expected detector response emerging from a collision or the source is described by the product of χ and χ^* [7], which leads to the integral equation:

$$\chi(\boldsymbol{r},E,\boldsymbol{\Omega})\chi^*(\boldsymbol{r},E,\boldsymbol{\Omega})=S(\boldsymbol{r},E,\boldsymbol{\Omega})\chi^*(\boldsymbol{r},E,\boldsymbol{\Omega})+$$

$$\int_{allV}\int_{4\pi}\int_{0}^{\infty}\chi(\boldsymbol{r}',E',\boldsymbol{\Omega}')\chi^*(\boldsymbol{r}',E',\boldsymbol{\Omega}')\frac{T(\boldsymbol{r}'\rightarrow\boldsymbol{r},E',\boldsymbol{\Omega}')\psi^*(\boldsymbol{r},E',\boldsymbol{\Omega}')}{\chi^*(\boldsymbol{r}',E',\boldsymbol{\Omega}')}\cdot$$

$$\frac{C(\boldsymbol{r},E'\rightarrow E,\boldsymbol{\Omega}'\rightarrow\boldsymbol{\Omega})\chi^*(\boldsymbol{r},E,\boldsymbol{\Omega})}{\psi^*(\boldsymbol{r},E',\boldsymbol{\Omega}')}dE'd\boldsymbol{\Omega}'dV' \tag{10}$$

It can be shown [8] that this modified transport process with a last event estimator leads to a zero variance Monte Carlo game, which means that all particles yield identical detector scores. If a collision estimator is used, Eq. (10) also leads to a zero variance game if the particle is not allowed to terminate [2].

The modified stochastic process of Eq. (10) can be written with a modified source density:

$$\tilde{S}(\boldsymbol{r}, E, \boldsymbol{\Omega}) = S(\boldsymbol{r}, E, \boldsymbol{\Omega})\chi^*(\boldsymbol{r}, E, \boldsymbol{\Omega}) \tag{11}$$

a modified transport kernel $\tilde{T}$:

$$\tilde{T}(\boldsymbol{r}' \to \boldsymbol{r}, E', \boldsymbol{\Omega}') = \frac{T(\boldsymbol{r}' \to \boldsymbol{r}, E', \boldsymbol{\Omega}')\psi^*(\boldsymbol{r}, E', \boldsymbol{\Omega}')}{\chi^*(\boldsymbol{r}', E', \boldsymbol{\Omega}')} \tag{12}$$

which is seen to be properly normalised by Eq. (8), and a modified collision kernel $\tilde{C}$:

$$\tilde{C}(\boldsymbol{r}, E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}) = \frac{C(\boldsymbol{r}, E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})\chi^*(\boldsymbol{r}, E, \boldsymbol{\Omega})}{\psi^*(\boldsymbol{r}, E', \boldsymbol{\Omega}')} \tag{13}$$

which is seen to be properly normalised by Eq. (9) with the detector response function put to zero (i.e. outside the detector phase space).

The modified transport kernel in the altered stochastic process given in Eq. (12) is seen to be biased with the event value ψ^* and the modified collision kernel given in Eq. (13) with the point value χ^*. From Eq. (11) it is seen that the modified source is also biased with the point value.

3 Implementation in the MORSE Monte Carlo Code

Biasing in MORSE as well as in other Monte Carlo codes, is done by modifying the PDFs of the transport process by means of importance functions given in the input. The aim of this section is to show what biasing methods are available in MORSE and how "good" values for the input parameters of these biasing methods can be derived. Although this section is specifically devoted to MORSE, many of the biasing methods are generally available in other Monte Carlo codes as well.

Because MORSE is a multigroup code and because the geometry is divided into zones each having its own biasing parameters, the importance functions are dependent on zone number and energy group. The intercollision distance of the particles is sampled from the PDF:

$$f(\eta_g) = \exp(-\eta_g) \tag{14}$$

where η_g is the optical thickness measured in mean free paths for energy group g. In MORSE the most favourable direction of particles is given in the input and the biased path length in that direction is sampled from the PDF:

$$f_1(\eta_g) = (1 - \mathrm{PATH}_{z,g})\exp\left[-(1 - \mathrm{PATH}_{z,g})\eta_g\right] \tag{15}$$

where $\mathrm{PATH}_{z,g}$ is an input parameter for zone number z and energy group g. This procedure corresponds to reducing the total cross section of the shield from Σ_{tg} to Σ^*_{tg} =

$(1 - \mathrm{PATH}_{z,g})\Sigma_{tg}$ in the most favourable direction. For other directions, $\mathrm{PATH}_{z,g}$ is multiplied with the cosine of the angle between the most favourable direction and the actual direction of the particle. This means for example that for directions of the particle opposite to the most favourable one, the path length is shrunk instead of stretched. It will now be shown how the best $\mathrm{PATH}_{z,g}$ value can be calculated [6].

As can be seen from Eq. (12) the transport kernel should be biased with the event value ψ^*. This implies that the biased PDF for path length selection should be:

$$f_2(\eta_g) = \frac{\psi^*(\eta_g) f(\eta_g)}{\int_0^\infty \psi^*(\eta_g) f(\eta_g) d\eta_g} = \frac{\psi^*(\eta_g)\exp(-\eta_g)}{\int_0^\infty \psi^*(\eta_g)\exp(-\eta_g) d\eta_g} \tag{16}$$

where $\psi^*(\eta_g)$ is the event value at a distance $r = \eta_g/\Sigma_{tg}$ away from the particle position for the energy group g of the current particle. PDF $f_2(\eta_g)$ in Eq. (16) is equal to PDF $f_1(\eta_g)$ in Eq. (15) if

$$\psi^*(\eta_g) = A_g \exp(\mathrm{PATH}_{z,g}\eta_g) \tag{17}$$

The MORSE input parameter $\mathrm{PATH}_{z,g}$ can thus be found by fitting an exponential through the event values as function of the optical distance from the source zone to the detector. All zones along that line will then have equal PATH values, but the PATH value can change from one group of zones to the other, and the index z can therefore not be omitted. Of course, the assumption that the event value will have a simple exponential form like Eq. (17) for each energy group implies that the transport kernel is not biased with the exact event value anymore, but with an exponential fit of the event value. But, as will be shown in Section 6, this assumption might be rather good.

In MORSE the selection of an energy group of source particles can be biased by Source Energy Biasing parameters (SEB) to be given in the input of the code for the source zone and each energy group. The PDF for energy group selection of source particles is then given by:

$$\tilde{S}_g(\mathbf{\Omega}) = \frac{S_g(\mathbf{\Omega})\mathrm{SEB}_g}{\sum_{g'=1}^{G} S_{g'}(\mathbf{\Omega})\mathrm{SEB}_{g'}} = \frac{S_g(\mathbf{\Omega})\chi^*_{s,g}}{\sum_{g'=1}^{G} S_{g'}(\mathbf{\Omega})\chi^*_{s,g'}} \tag{18}$$

where s is the source zone number, G the total number of energy groups and S_g the natural source spectrum. From Eq. (11) it is seen that the point values of the source zone should be used for the SEB input parameters. Note that the angular averaged point value is used for this purpose, and not the angular dependent point value as one would expect from Eq. (11). Using the angular dependent point value would complicate the input of the code notably.

Also the energy group of particles emerging from a collision can be biased in MORSE. This is done by means of Energy Biasing at Collision parameters (EBC) to be given in the input of the code for each zone and each energy group. The energy group of emerging particles is than given by:

$$\tilde{C}_{z,g} = \frac{C_{z,g}\mathrm{EBC}_{z,g}}{\sum_{g'=1}^{G} C_{z,g'}\mathrm{EBC}_{z,g'}} = \frac{C_{z,g}\chi^*_{z,g}}{\sum_{g'=1}^{G} C_{z,g'}\chi^*_{z,g'}} \tag{19}$$

From Eq. (13) it is seen that the point values of each zone and energy group should be used for the EBC input parameters. Again the angular averaged point values are used for

this purpose and not the angular dependent ones. After selection of the energy group of the emerging particle, its direction is sampled.

The last biasing procedures applied in the calculations are Russian roulette and splitting. These biasing schemes are also applied to particles emerging from a collision. In fact Russian roulette does not lead to lower variances, but to less CPU time spent per particle. The overall effect is that the "Figure of Merit" defined by:

$$\text{FoM} = \frac{1}{\sigma^2 T_{CPU}} \tag{20}$$

where σ is the fractional standard deviation of the calculation and T_{CPU} the spent CPU time, increases if the parameters for Russian roulette and splitting are set properly.

Russian roulette and splitting is set by a "weight window" for each zone and energy group. The weight window for a specific zone and group is set by the upper limit WTHI, the lower limit WTLO and the survival weight WTAV. If the particle emerges from a collision with weight above WTHI, the particle is split into two particles with each one half of the initial particle weight. If the two remaining particles still have a weight higher than WTHI, the two particles are both split again. This process goes on until the particles have weights lower than WTHI. If a particles emerges from a collision with weight below WTLO, it is rouletted and gets a weight WTAV upon survival. Of course the survival probability in the roulette game is such that the process is unbiased, i.e. that on the average no weight is absorbed or no extra weight is introduced in the calculation. Both WTHI, WTLO and WTAV must be determined beforehand in the input of the MORSE code for each zone and energy group.

There are no general rules to determine WTHI, WTLO and WTAV of each zone and energy group, because these values are rather dependent on the problem under consideration. However, it seems natural to choose WTHI, WTLO and WTAV as functions of the point values of each zone and energy group. Using Russian roulette and splitting implies that the particles in a specific zone z and energy group g have weights between $\text{WTLO}_{z,g}$ and $\text{WTHI}_{z,g}$. $\text{WTAV}_{z,g}$ is the survival weight of Russian roulette, and should have a value between WTLO and WTHI (a value lower than WTLO would make no sense because the Russian roulette survival probability would always be zero, and a value above WTHI would make no sense either because a particle surviving Russian roulette would directly be split into two particles again). $\text{WTAV}_{z,g}$ should therefore be a kind of average particle weight in a logarithmic sense:

$$\text{WTLO}_{z,g} = \frac{\text{WTAV}_{z,g}}{f} \text{ and } \text{WTHI}_{z,g} = \text{WTAV}_{z,g} f \tag{21}$$

where f is a factor ($f > 1$) which should have a value such that particles which are rouletted in a particular zone are not directly split in the neighbouring zone and vice versa, because this would lead to a waste of CPU time. The value of f is therefore another parameter to be optimized.

It was shown [1] that in near optimal calculations particle weights are inversely proportional to the point value. If $\text{WTAV}_{z,g}$ is interpreted as the "average" particle weight of zone z and group g, it can be written as a function of the point values along the line from source to detector:

$$\text{WTAV}_{z,g} = \frac{S_g}{\bar{S}_g} \frac{\chi^*_{s,g}}{\chi^*_{z,g}} \tag{22}$$

where S_g and $\tilde{S}_g$ are the original and biased PDFs for source energy group selection and $\chi^*_{s,g}$ and $\chi^*_{z,g}$ are the point values of the source zone s and shield zone z, respectively. If no source energy biasing is used, the average weight is just equal to the ratio of the point values of the source zone s and the shield zone z, and if source energy biasing is used, the average weight of the source is just equal to the ratio of S_g and $\tilde{S}_g$, as it should be to have a fair Monte Carlo biasing.

It must be noted here that other methods exist specifically devoted to optimizing parameters for (surface) splitting. The optimization of splitting parameters according to the DSA method is described in Ref. 9.

4 Calculation of Point Values

The aim of this section is to derive an expression for the point value of a specific zone and energy group, which can be used in a subsequent Monte Carlo shielding calculation to set the weight window for that zone or group.

A particle entering a specific zone and group will be rouletted or split if its weight is outside the weight window. In a shielding calculation, it is likely that Russian roulette or splitting happens only the first time the particle emerges from a collision in that zone and group, because the weight of the particle during all further collisions is only reduced by the non-absorption probability, which is a number fairly close to unity (for concrete the non-absorption probability is larger than 0.93 for all energies ranging from thermal to fast). As the first collision in a specific zone and group is the most important one with respect to Russian roulette and splitting, it makes sense to calculate point values averaged over a zone and group, which are weighted by the firstly emitted particle density. This is the density of particles in a zone and group emitted either from the source or from collisions while their previous collision was in another zone and/or group:

$$\chi^*_{z,g} = \frac{\text{Total detector score of firstly emitted particles in (z,g)}}{\text{Total weight of firstly emitted particles in (z,g)}} \tag{23}$$

Point of departure to derive such point values will be the integral transport equations for the emergent particle density and the point value. Eqs. (1) and (4) are slightly rewritten to:

$$\chi(\boldsymbol{P}) = S(\boldsymbol{P}) + \int_{\Gamma} \chi(\boldsymbol{P}')L(\boldsymbol{P}' \rightarrow \boldsymbol{P})d\boldsymbol{P}' \tag{24}$$

$$\chi^*(\boldsymbol{P}) = h(\boldsymbol{P}) + \int_{\Gamma} \chi^*(\boldsymbol{P}')L(\boldsymbol{P} \rightarrow \boldsymbol{P}')d\boldsymbol{P}' \tag{25}$$

where $L(\boldsymbol{P} \rightarrow \boldsymbol{P}')$ is the total transport kernel (see Eq. (1)) for transport from $\boldsymbol{P}$ to $\boldsymbol{P}'$, with $\boldsymbol{P}$ and $\boldsymbol{P}'$ being the six-dimensional scalar coordinates of the particles. The integration of both equations extends over the whole phase space Γ, which is supposed to consist of two mutually exclusive subspaces Γ_s and Γ_p such that $\Gamma_s + \Gamma_p = \Gamma$. Multiplying each term of Eq. (25) by $\chi(\boldsymbol{P})$ and integrating over Γ_s (this subspace will be defined later) yields:

$$\int_{\Gamma_s} \chi(\boldsymbol{P})\chi^*(\boldsymbol{P})d\boldsymbol{P} =$$

$$= \int_{\Gamma_s} \chi(\boldsymbol{P}) h(\boldsymbol{P}) dP + \int_{\Gamma} \left[\int_{\Gamma_s} \chi(\boldsymbol{P}) L(\boldsymbol{P} \rightarrow \boldsymbol{P}') dP \right] \chi^*(\boldsymbol{P}') dP' \tag{26}$$

where the integration order of $\boldsymbol{P}$ and $\boldsymbol{P}'$ has been reversed in the second term on the RHS. The term between the square brackets on the RHS of Eq. (26) is the number of particles emerging from a collision at $\boldsymbol{P}'$ per unit phase space, which were emitted previously in Γ_s. A shorthand notation for this number will be:

$$\int_{\Gamma_s} \chi(\boldsymbol{P}) L(\boldsymbol{P} \rightarrow \boldsymbol{P}') dP = [\chi(\boldsymbol{P}')]_{\Gamma_s} \tag{27}$$

The second term on the RHS of Eq. (26) is now split into two parts:

$$\int_{\Gamma} [\chi(\boldsymbol{P}')]_{\Gamma_s} \chi^*(\boldsymbol{P}') dP' = \int_{\Gamma_s} [\chi(\boldsymbol{P}')]_{\Gamma_s} \chi^*(\boldsymbol{P}') dP' + \int_{\Gamma_p} [\chi(\boldsymbol{P}')]_{\Gamma_s} \chi^*(\boldsymbol{P}') dP' \tag{28}$$

Eq. (28) is substituted in Eq. (26) and the first part of the RHS of Eq. (28) is transported to the LHS of Eq. (26). One then obtains:

$$\int_{\Gamma_s} \left(\chi(\boldsymbol{P}) - [\chi(\boldsymbol{P})]_{\Gamma_s} \right) \chi^*(\boldsymbol{P}) dP = \int_{\Gamma_s} \chi(\boldsymbol{P}) h(\boldsymbol{P}) dP + \int_{\Gamma_p} [\chi(\boldsymbol{P})]_{\Gamma_s} \chi^*(\boldsymbol{P}) dP \tag{29}$$

We will now specify the subspace Γ_s as the volume of a geometrical zone z, the energy span of group g and the whole angular space 4π. To define an average point value for zone z and group g, Eq. (29) is written as:

$$\chi^*_{z,g} \int_{\Gamma_s} \left(\chi(\boldsymbol{P}) - [\chi(\boldsymbol{P})]_{\Gamma_s} \right) dP = \int_{\Gamma_s} \chi(\boldsymbol{P}) h(\boldsymbol{P}) dP + \int_{\Gamma_p} [\chi(\boldsymbol{P})]_{\Gamma_s} \chi^*(\boldsymbol{P}) dP \tag{30}$$

so that:

$$\chi^*_{z,g} = \frac{\int_{\Gamma_s} \left(\chi(\boldsymbol{P}) - [\chi(\boldsymbol{P})]_{\Gamma_s} \right) \chi^*(\boldsymbol{P}) dP}{\int_{\Gamma_s} \left(\chi(\boldsymbol{P}) - [\chi(\boldsymbol{P})]_{\Gamma_s} \right) dP} \tag{31}$$

Each term of Eq. (30) has a plain physical meaning. $\chi^*_{z,g}$ is the point value of zone z and group g, the integral on the LHS is the firstly emitted particle density (the total weight of particles emitted in zone z and group g, minus the weight of particles emitted previously in zone z and group g; particles contributing to this density may have emerged from a collision in zone z and group g before, but not directly before their last emission in zone z and group g). The first term on the RHS is the expected detector response of particles emitted in zone z and group g, and the second term on the RHS is the expected detector response of particles, which had their previous emission in zone z and group g. From Eq. (31) it is seen that $\chi^*_{z,g}$ is properly weighted by the firstly emitted particle density. Note that the point values thus obtained, are not only averaged over the volume of zone z and the energy span of group g, but also over the whole angular space 4π. They can therefore directly be used to calculate the SEB and EBC input parameters of Eqs. (18) and (19).

The same derivation as above can be given for the event value and one obtains:

$$\psi^*_{z,g} \int_{\Gamma_s} \left(\psi(\boldsymbol{P}) - [\psi(\boldsymbol{P})]_{\Gamma_s}\right) dP = \int_{\Gamma_s} \psi(\boldsymbol{P}) g(\boldsymbol{P}) dP + \int_{\Gamma_p} [\psi(\boldsymbol{P})]_{\Gamma_s} \psi^*(\boldsymbol{P}) dP \qquad (32)$$

where g is the detector response function for the collision density $\psi(\boldsymbol{P})$, and $\psi^*_{z,g}$ is the event value of zone z and group g.

The integral on the LHS of Eq. (32) is the firstly collided particle density (the total weight of particles entering a collision in zone z and group g, minus the weight of particles collided previously in zone z and group g; particles contributing to this density may have entered a collision in zone z and group g before, but not directly before their last collision in zone z and group g). The RHS of Eq. (32) is again the sum of the expected detector response of particles entering a collision in zone z and group g and the expected detector responses of particles, wich had their previous collision in zone z and group g.

For the calculation of χ^*, the weight of particles emerging from a collision is used as a weighting factor, while for ψ^* the weight of particles entering a collision is used. Because the non-absorption probability is close to one (at least for concrete), the zone averaged point value and event value for a specific energy group will not differ very much. The relation between the event value and the point value outside the detector phase volume (zero detector response function) can be derived from Eq. (9) and reads [7]:

$$\psi^*_g(\boldsymbol{r}, \boldsymbol{\Omega}) = \sum_{g'} \int_{4\pi} \frac{\Sigma^g_s(\boldsymbol{r})}{\Sigma^g_t(\boldsymbol{r})} \frac{\Sigma^{g \to g'}_s(\boldsymbol{r}, \boldsymbol{\Omega} \to \boldsymbol{\Omega}')}{\Sigma^g_s(\boldsymbol{r})} \chi^*_{g'}(\boldsymbol{r}, \boldsymbol{\Omega}') d\Omega' \qquad (33)$$

The relation between the angular integrated value functions for a simple one speed problem outside the detector phase volume then reads:

$$\psi^*(\boldsymbol{r}) = \int_{4\pi} \psi^*(\boldsymbol{r}, \boldsymbol{\Omega}) d\Omega =$$

$$= \int_{4\pi} \int_{4\pi} \frac{\Sigma_s(\boldsymbol{r})}{\Sigma_t(\boldsymbol{r})} \frac{\Sigma_s(\boldsymbol{r}, \boldsymbol{\Omega} \to \boldsymbol{\Omega}')}{\Sigma_s(\boldsymbol{r})} \chi^*(\boldsymbol{r}, \boldsymbol{\Omega}') d\Omega' d\Omega = \frac{\Sigma_s(\boldsymbol{r})}{\Sigma_t(\boldsymbol{r})} \chi^*(\boldsymbol{r}) \qquad (34)$$

where it is assumed that the scattering cross section is only dependent on the cosine of the scattering angle $\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}'$ (but not necessarily isotropically). From Eq. (34) it is seen that the two value functions differ only by the non-absorption probability. When the value functions described above are calculated by a Monte Carlo code, the statistical uncertainties are expected to be much larger than the differences between the two value functions. For practical purposes, therefore, it is sufficient to calculate only one of the two value functions, and to set the event value and point value equal to each other for each zone and group.

The above mentioned method can easily be implemented in the MORSE-SGC/S Monte Carlo code, although this method imposes some restrictions on the number of progenies a particle can create and the number of energy groups and zones. Also no use can be made of the supergrouping facility because of bookkeeping difficulties, so older versions of the MORSE code can be used as well. The weight of each firstly emitted particle is added to a WEIGHT array, which contains the sum of the weights of such particles per zone and group.

Note that a particle which emerges from the source or a collision in zone z and group g, enters another zone and/or group, scatters to zone z and group g again and emerges from a collision there, is counted twice. In that case, however, the detector contribution of that particle must be counted twice, too. Therefore, a NUMBER array is bookkeeped, which contains the number of times a particle contributes this way. Each time a particle or one of its progenies scores in the detector, its score is multiplied by the NUMBER array and added to a SCORE array, which contains the sum of all scores of each zone and group. At the end of the Monte Carlo calculation, the WEIGHT and SCORE arrays are written to a file, which can be read again when the Monte Carlo calculation is restarted. Dividing the elements of the SCORE array by the corresponding elements of the WEIGHT array gives the estimate of the point value of each zone and group, which can be used to bias the PDFs and to calculate the weight window and the exponential transform parameter for each zone and group.

5 Calculation of Importance Functions

If the point value is known for each zone and each energy group, the input parameters for the importance biasing methods can be calculated [6]. As shown in Section 3, the calculated point values of the source zone can directly be used to bias the PDF for source energy group selection. The SEB input parameters are derived from Eq. (18). The point values of each zone can be used to bias the PDF for energy group selection at collision sites. The EBC input parameters are derived from Eq. (19).

According to Eq. (22), the Russian roulette survival weight for each zone and energy group ($\mathrm{WTAV}_{z,g}$) is taken inversely proportional to the point value of that zone and group. This implies that all contributing particles have similar weights, which is likely to reduce the variance of the scores of the non-zero contributing particles. The weight limits below which Russian roulette will be invoked (WTLO) and above which splitting will occur (WTHI), can be set as a function of the WTAV value of that zone and energy group (see Eq. (21)), or as a function of the WTAV values of neighbouring zones. The influence of the value of f introduced in Eq. (21) is further investigated in the example in Section 6.

According to Eq. (17) (and shown earlier [6]), the input parameter for exponential biasing can be calculated by fitting an exponential function through the event values as function of the optical thickness from the source zone to the detector. For reasons explained earlier, the point value is used here instead of the event value, which does not abuse the method in an essential fashion. Along the line from source to detector, one obtains for the fitted point value of zone z and group g:

$$\chi^*_{z,g} = A_g \exp\left(C_g \int_0^{D_z} \Sigma_t^g(s)\, ds\right) \tag{35}$$

where D_z is the distance from the source zone to the center of zone z. This distance can be calculated in different ways. For example, the center of the source zone can be calculated by averaging over all particle source coordinates, the center of each zone can be calculated by averaging over all particle collision coordinates, and the distance from the source zone to the shield zone can be taken as the difference of these averaged coordinates. Intuitively this

seems a good procedure. Practically speaking, however, this may be cumbersome because it needs extra programming in the Monte Carlo code Therefore, in the example of Section 6 where a plane source is used, the distance from the source plane to the geometrical center of each zone is used for D_z.

For each zone and group, the total cross section and the point value is known, so the fitting parameters A_g and C_g can be obtained. This is done by a linear least squares method. Taking the logarithm of Eq. (35) and writing $\eta_{z,g}$ for the optical thickness from the source zone s to shield zone z, one gets for the sum of squared deviations:

$$\epsilon^2 = \sum_z \left(\ln(\chi^*_{z,g}) - \ln(A_g) - C_g\,\eta_{z,g}\right)^2 \tag{36}$$

where the summation is over each zone along the line from source to detector. Setting the derivatives of the RHS of this equation with respect to $\ln(A_g)$ and C_g to zero, leads to two expressions for these two fitting parameters. From Eqs. (17) and (35) it is seen that C_g can directly be used for the values of $\mathrm{PATH}_{z,g}$ for all zones along the line from the source to the detector.

As stated before, the point values calculated according to Section 4, are likely to suffer from large statistical variations. If it is seen that the point values fluctuate considerably from one energy group to another, they can be smoothed somewhat by collapsing energy groups together. This is done by taking the sum of the SCORE array for these groups and the sum of the WEIGHT array, and using the ratio of these two sums as the average point value for the energy groups collapsed together. In fact, this is the same as taking a weighted average of the point values of these energy groups. If groups G' to G'' are collapsed to one group G, one obtains for the average point value:

$$\chi^*_{z,G} = \sum_{g=G'}^{G''} \left(\frac{W(z,g)}{\sum_{g'=G'}^{G''} W(z,g')} \frac{S(z,g)}{W(z,g)} \right) = \frac{\sum_{g=G'}^{G''} S(z,g)}{\sum_{g=G'}^{G''} W(z,g)} \tag{37}$$

where W and S are shorthand notations for the values of the WEIGHT and SCORE arrays, respectively. The $\chi^*_{z,G}$ value thus obtained is taken the same for each energy group ranging from G' to G''. The validity of this procedure can easily be seen from Eq. (30). As the subspace Γ_s can be chosen arbitrarily, it can contain the energy range of several energy groups together instead of only one.

If the point values fluctuate from one zone to another, they can be smoothed by using point values calculated from the fitting parameters A_g and C_g in Eq. (35). It must be emphasized that the original and smoothed values should be compared carefully, because wrong value functions will only worsen the efficiency of the Monte Carlo calculation instead of improving it.

6 Example

The method can best be illustrated by an example. In Fig. 1, the geometry of a straight cylindrical duct in concrete with a 1 cm thick steel liner is shown. A plane source calculated

by the DOT3.5 code [10] in 25 energy groups and P_3S_8 mode, and converted to MORSE-SGC/S format by the DOMINO code [11], irradiates the duct with length of 100 cm and radius of 5 cm. This duct is almost similar to the one for which this method was originally developed and for which measurements were performed [12]. A boundary crossing detector, which is equally sensitive to all energy groups and which measures the particle flux, is positioned at the end of the duct. The zones are positioned concentric around the duct at equi-distant distances and numbered from 1 to 40 (zones 1 to 10 are steel, 11 to 40 concrete). Each zone has its own set of biasing parameters accompanied.

The first calculation is done by manual setting of biasing parameters (WTAV, WTLO, WTHI and PATH). Neither source energy biasing, nor energy biasing at collision sites are used in this calculation because of the lack of knowledge of point values. The WTAV of zone 1 is 1.0, and is divided by 2 for each zone along the axial direction and multiplied by 2 for each zone along the radial direction, as shown in the lower half of Fig. 1. In the first calculation, PATH is 0.5 in axial direction towards the detector for all groups and all zones (note that these values of WTAV and PATH are quite arbitrary).

The point values obtained from the first calculation are averaged over fast ($E > 1.0$ MeV), intermediate (0.4 eV $\leq E \leq$ 1.0 MeV) and thermal groups ($E <$ 0.4 eV), according to Eq. (37), and an exponential fit according to Eq. (35) is used to smoothen the spatial behaviour of the point values. The point values for energy group 3 (1.0–2.23 MeV) and energy group 23 (0.025–0.05 eV) for the three concrete layers are shown in Figs. 2 and 3, respectively. It is noted that, although groups 1 to 3 have equal point values for each zone due to smoothing according to Eq. (37), the point value as a function of optical distance for each group is different due to different cross sections of each group. The same is true of course for the other groups smoothed together. The optical distance in Figs. 2 and 3 is measured parallel to the duct axis from the detector plane (at 100 cm in Fig. 1), to the center of each shield zone. From Figs. 2 and 3, it is seen that the exponential fit, necessary to determine the exponential transform parameter C_g in Eq. (35), is quite reasonable. Discrepancies between the point values and the exponential fit can be seen only for small distances. This might be caused by the fact that the distance from the detector to the center of each zone is measured parallel to the duct axis, and not along the line from the center of the detector to the center of each zone. This leads to a relatively large overestimation of the zone-detector distance for zones close to the detector, and is a major point to improve in the programming of this method.

The weights of the source particles and the WTAV and PATH values for all zones and energy groups for the subsequent calculations are calculated from the point values according to Section 5. The weights of the source particles for the fast, intermediate and thermal groups are given in Fig. 4 within the source plane. It is seen that the weights of the fast energy groups are reduced from 1 to 0.41, which resembles the fact that fast neutrons are sampled about 2.5 times more than in the first calculation as these neutrons have a higher probability to reach the detector due to lower cross sections. However, the weights of the thermal neutrons are increased from 1 to 3.95, which implies that thermal source neutrons are sampled about 4 times less.

The WTAV values are shown in the lower half of Fig. 4 for the three concrete layers for the fast, intermediate and thermal energy range. It is seen that the ratio of WTAV values of two neighbouring zones is about 2 in axial direction for all energy groups, and a factor

of 2 to 3 in radial direction for the fast groups and about 3 to 4 in radial direction for the thermal groups.

This implies that the original WTAV values used for calculation 1 were already quite good. In the upper half of Fig. 4 the values of PATH for energy groups 3 and 23 are given. Note that the values of PATH for each energy group are equal for all zones of one shield layer (i.e. zones 11 to 20, 21 to 30 and 31 to 40). It is seen from this figure that the PATH values hardly change from one concrete layer to the other. This follows also from Figs. 2 and 3, where it is seen that the slope of the curves for each energy group are almost equal for all three concrete layers. Because PATH is larger for higher energies, the exponential transform is more effective for fast neutrons.

The point values obtained from the first calculation, were not only used for the calculation of the biasing parameters for the weight window and exponential transform (the WTAV and PATH parameters), but also for the calculation of the biasing parameters for source energy biasing and energy biasing at collision sites (the SEB and EBC values). Because the point values were averaged over fast, intermediate and thermal groups, only crude energy biasing could be performed. The values of A_g in Eq. (35) of the point values in the steel liner (zones 1 to 10 in Fig. 1), were used for the point values of the source particles.

A short overview of all calculations performed is given in Table 1, while the collided fluxes of the calculations are given in Table 2. From Table 2, it is seen that the Figures of Merit of calculations 2 to 7 are much higher than those of calculation 1, resembling the fact that calculations 2 to 7 are much more efficient. This is especially true for the fast and intermediate fluxes, whose Figures of Merit are increased with a factor of 2 to 3. This is to be expected of course, because not only the weight window limits and the path length stretching parameters were set more properly in calculations 2 to 7, but also the parameters for Source Energy Biasing and Energy Biasing at Collision sites were set in these calculations, while these biasing methods were not used in the first calculation. Especially the use of Source Energy Biasing is expected to lead to lower variances for the fast and intermediate fluxes because fast neutrons are sampled about 2.5 times more, as can be seen from Fig. 4. The increase of efficiency of calculations 2 to 7 depends of course on the initial WTAV, WTLO, WTHI and PATH values used in the first run. As can be seen by comparing Figs. 1 and 4, these values for the first run were already quite good. Hence, the improvements due to the importance sampling would be (much) larger if the setting of the parameters for the Russian roulette and splitting for the first run did not coincidentally fit so nicely to this problem.

Generally it can be seen that the calculations with weight window width (f value) of 2 to 5 are the most efficient ones, and that calculations using path length biasing are more efficient than calculations without path length biasing.

The point values used for calculations 2 to 7 were obtained from calculation 1, which used about 89 hours of CPU time. It was found, however, that the PATH value obtained from the exponential fit through the point values (see Eq. (35)) converged much faster. Therefore, it is possible to calculate point values already after a few hours of CPU time instead of 89 hours, and to do Monte Carlo calculations with biasing input parameters calculated from the obtained point values. This can even be done in an interative way to minimize CPU times.

7 Conclusions

To improve the efficiency of Monte Carlo calculations, knowledge of the important parts of the shield and energy range is necessary, to bias the Monte Carlo calculations properly. The point values of each zone and energy group can be estimated from a forward Monte Carlo run, and it is shown that subsequent Monte Carlo runs can be much more efficient if these point values are used to bias these runs. The point values can be updated during the subsequent Monte Carlo calculations, leading to continuously improving biasing parameters.

To smoothen the point values estimated in a first Monte Carlo run over energy and space, considerable programming is necessary, which depends on the problem under consideration, and which requires a thorough knowledge of the code used. A considerable portion of this programming can be avoided by using only energy averaged point values. Care must be taken in this case to ensure that the estimated point values are non-zero for each zone.

A general applicable and fully automized biasing procedure, is difficult to establish because of the above mentioned problems. However, if the method is applied to specific classes of shielding problems (e.g. straight ducts, bent ducts, spent fuel casks), the programming has to be done only once for each class, and a large increase of efficiency may be attained.

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Table 1: Biasing parameters for the calculations. The point values for calculations 2 to 7 are obtained from the first calculation, and are averaged over fast, intermediate and thermal groups. SEB means source energy biasing, EBC energy biasing at collision sites. f is the ratio between WTHI and WTAV. The CPU time is given in hours on a VAX 4090 workstation.

Calc	CPU	WTAV	f	PATH	SEB	EBC
1	89.2	input[a)]	10	0.5	no	no
2	28.9	autom.	2	autom.	autom.	autom.
3	25.5	autom.	5	autom.	autom.	autom.
4	23.6	autom.	10	autom.	autom.	autom.
5	30.2	autom.	2	no	autom.	autom.
6	24.1	autom.	5	no	autom.	autom.
7	25.1	autom.	10	no	autom.	autom.

[a)] See Fig. 1 for the actual values.

Table 2: Collided fast, intermediate, thermal and total fluxes per unit source strength in units of 10^{-7} cm^{-2} s^{-1}. The numbers between parenthesis are the percentage standard deviation. The Figure of Merit (FoM) is defined according to Eq. (20).

Calc	f	Fast Flux	FoM	Interm. Flux	FoM	Thermal Flux	FoM	Total Flux	FoM
1	10	2.34 (3.2)	11.0	5.19 (2.2)	23.2	2.70 (2.9)	13.3	10.22 (1.5)	49.8
2	2	2.55 (3.8)	24.0	5.02 (2.4)	60.1	2.31 (5.5)	11.4	9.88 (2.1)	78.5
3	5	2.49 (4.0)	24.5	5.13 (2.7)	53.8	2.67 (5.7)	12.1	10.28 (2.2)	81.0
4	10	2.45 (4.5)	20.9	4.92 (3.1)	44.1	2.84 (7.5)	7.5	10.21 (2.7)	58.1
5	2	2.46 (3.8)	22.9	5.13 (2.4)	57.5	2.63 (5.7)	10.2	10.22 (2.2)	68.4
6	5	2.41 (4.2)	23.5	5.12 (3.1)	43.2	2.67 (6.6)	9.5	10.20 (2.5)	66.4
7	10	2.40 (4.4)	20.6	5.16 (2.9)	47.4	2.35 (7.2)	7.7	9.87 (2.5)	63.7

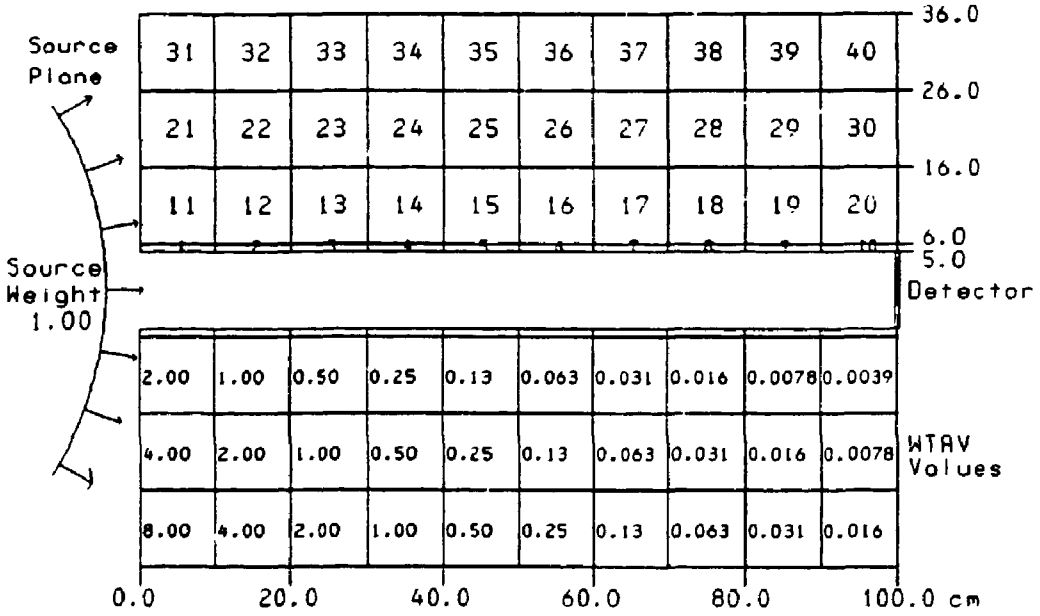

Figure 1: Horizontal cross section of the straight duct in concrete with a 1 cm thick steel liner. The zone numbers are given in the upper half of the duct, the WTAV values for the first three calculations in the lower half. Regions 1 to 10 are made of steel, 11 to 40 of concrete. The weights of all the source particles are unity. The flow rate distribution through a cylinder plane acts as the source.

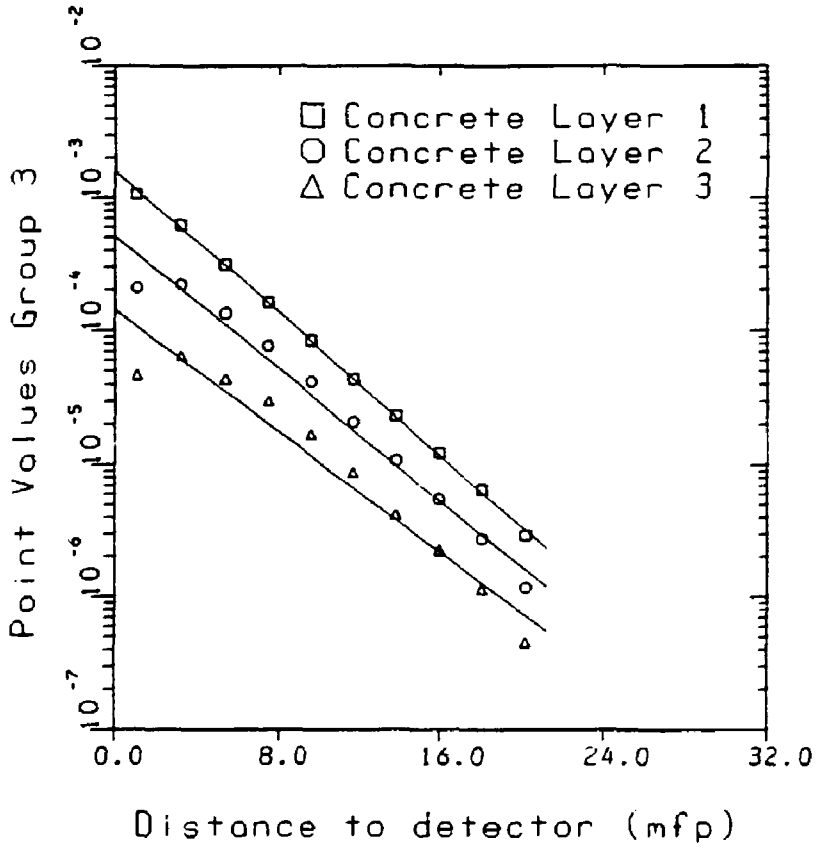

Figure 2: Point values for group 3 (1.0–2.23 MeV) as a function of the optical shield thickness from the detector plane to the center of each zone along the duct axis. These values are calculated from the first MORSE-SGC/S calculation. The solid line is the linear least squares fit.

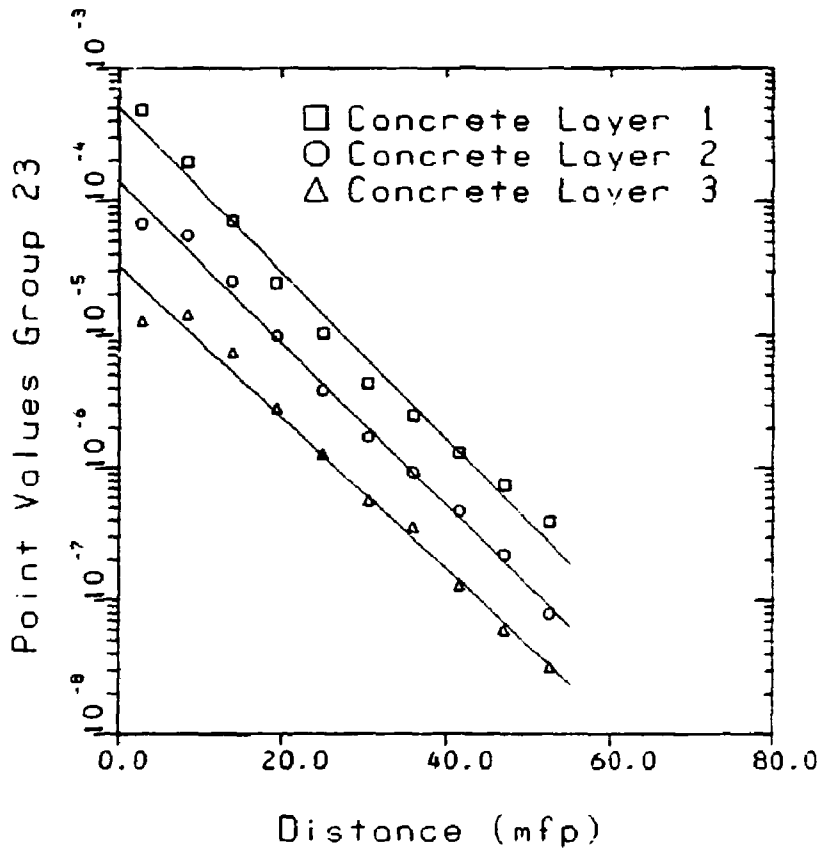

Figure 3: Point values for group 23 (0.025–0.05 eV) as a function of the optical shield thickness from the detector plane to the center of each zone along the duct axis. These values are calculated from the first MORSE-SGC/S calculation. The solid line is the linear least squares fit.

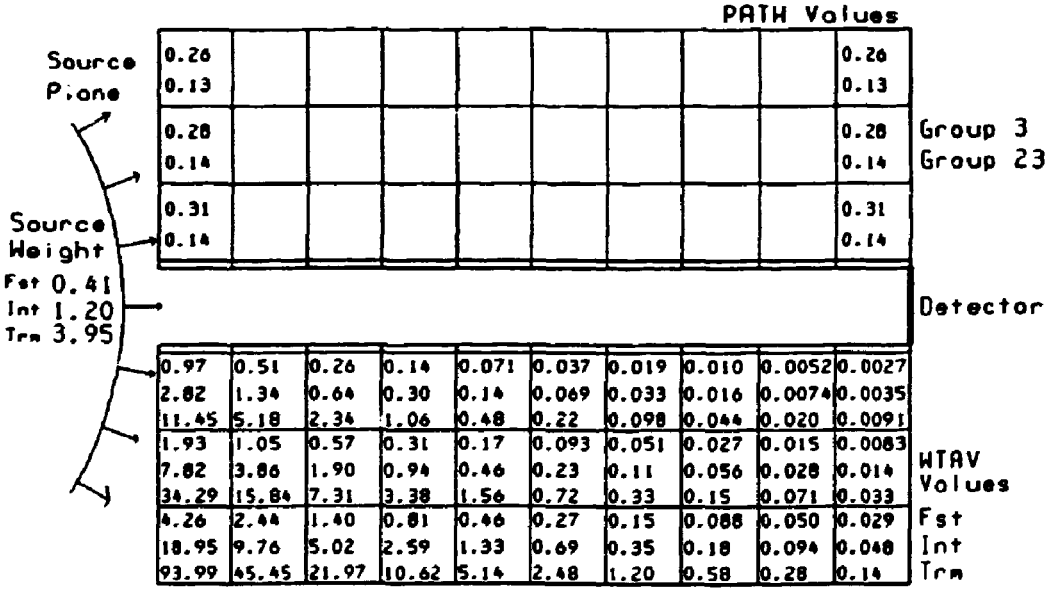

Figure 4: Horizontal cross section of the straight duct in concrete with a 1 cm thick steel liner. The PATH values for calculations 2 to 7 are given in the upper half of the duct, the WTAV values in the lower half. The PATH values for each energy group are the same for all zones of one shield layer. The weights of the source particles and the WTAV values are given for fast (Fst), intermediate (Int) and thermal (Trm) groups.