Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

IMPACT OF IMPORTANCE QUALITY IN COUPLED ELECTRON-PHOTON-POSITRON SIMULATION USING SPLITTING/ROULETTING VR TECHNIQUES

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ABSTRACT

The detailed simulation of the full electron-photon cascade may require large computational resources to obtain adequate statistics in a reasonable amount of time. Therefore, the study of variance reduction techniques for this class of problem is necessary. This paper studies the impact of the quality of the importance function (with a specific focus on deterministic importance function) used for transport biasing in a coupled electron-photon-positron Monte Carlo simulation using splitting/rouletting variance reduction techniques. More specifically, this work addresses the issue of the degradation of the performance and accuracy when explicit positron biasing is not performed for such methodologies.

Key Words: Variance reduction, Deterministic importance, Coupled electron-photon-positron

1. INTRODUCTION

Monte Carlo (MC) coupled electron-photon-positron transport calculations are often performed to determine characteristics such as energy or charge deposition in various types of devices. The detailed simulation of the full electron-photon cascade may require large computational resources in order to obtain adequate statistics in a reasonable amount of time, especially in complex three-dimensional geometries. Therefore, the study of variance reduction (VR) techniques for this class of problem is necessary.

In our previous work [1], the ADEIS (Angular-dependent adjoint Driven Electron-photon Importance Sampling) VR methodology was introduced. It was shown that ADEIS, which uses an angular/space/energy deterministic importance-based weight-window, produces significant speedups for coupled electron-photon-positron simulation. However, it was also shown that the quality of the importance functions can seriously impact the performance and accuracy of the methodology. Note that by an importance function of good quality, we refer to a function that has all the desirable characteristics to produce accurate and statistically well behaved tallies when used for transport biasing in ADEIS. A few parameters such as energy group structure, spatial meshing, objective selection and positron biasing can also affect the quality of the importance function. However, this paper presents only studies related to explicit positron biasing because of its large impact on the accuracy of the simulation.

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2. ADEIS METHODOLOGY

The ADEIS methodology is derived from the CADIS (Consistent Adjoint Driven Importance Sampling) methodology [2] which combines source and transport biasing within the MCNP weight-window technique [3]. This section presents a brief overview of the specific features of ADEIS and a short review of some useful concepts.

2.1. ADEIS Specific Features

A large class of problems requiring electron-photon-positron transport involves beam sources that are often considered mono-energetic. Since the expected gain from performing source biasing for such problems is minimal (even zero in the case of a mono-energetic pencil beam), the current ADEIS methodology only performs transport biasing. However, the statistical weight of the source particles is adjusted in order to preserve the consistency between the source and the weight-window. In order to automate the overall process, a new command line option and a new card were added to MCNP5.

This new MCNP5 simulation sequence begins similar to the standard sequence by the input file (imcn) and cross-section (xact) processing. However, before performing the transport calculation (mcrun), information such as material boundaries and compositions are extracted. At this point, the ADEIS shared library is called to perform a deterministic sequence defined in the ADEIS input file. At the end of this sequence, a modified version of the standard *wwinp* file is generated and control is returned to MCNP5, where the biased transport simulation is performed. Fig. 1 shows the different steps involved in the automated ADEIS simulation.

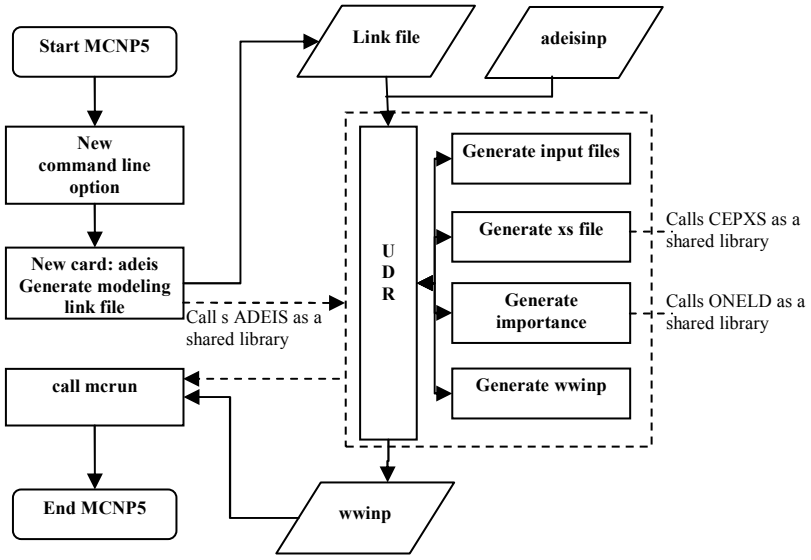

Figure 1 Automated ADEIS Flow Chart

2.1.1. Line of sight approach

Due to the impractical computational cost[1] associated with performing 3D deterministic transport simulation for coupled electron-photon-positron problems, the current version of ADEIS uses 1D transport simulation to obtain the importance functions. In order to automatically generate applicable 1D importance functions, a "line of sight" approach is introduced.

In this approach, the user defines a "line of sight" in the direction of the beam and a 1D model is generated along that line. However, this approach is mainly suited for problem types in which the beam is relatively well collimated.

2.1.2. Angular/space/energy lower-weight bounds

Since problems with beam sources are considered and because electrons (as well as the secondary photons) are scattered mainly in the "forward" direction, the resultant flux distributions are highly angular dependent. Therefore, to achieve a higher efficiency, it is expected that the bounds of the weight-window should be angular dependent in addition to the typical space and energy dependencies [2]. To address this issue in the context of this deterministic importance-based VR, the lower-weight bounds are based on angular importance integrated within a field-of-view subtending the region of interest (ROI) as illustrated in Fig. 2.

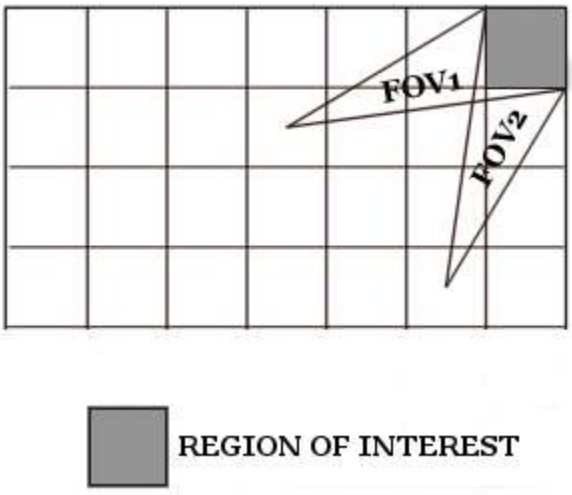

Figure 2 Spatially-Dependant Field-of-View (FOV)

[1] Large number of energy groups and angular moments, high quadrature, and possible upscattering

Mathematically, these lower-weight bounds are evaluated using the following formulations,

$$w_{L,\pm}(\vec{r},E) = \frac{R}{\varphi^{\dagger}_{\pm}(\vec{r},E)\,c}, \tag{1}$$

where,

$$\varphi^{\dagger}_{\pm}(\vec{r},E) = \int\limits_{\substack{+:\Omega\in FOV\\ -:\Omega\notin FOV}} d\Omega\,\Omega\,\psi^{\dagger}(\vec{r},E,\Omega), \tag{2}$$

c is user-defined constant, R is the response for a problem with an incoming flux at the boundary as follows,

$$\mathbf{R} = \int_{\Gamma} \mathbf{d\Gamma} \int \mathbf{dE} \int\limits_{\hat{\mathbf{n}}\cdot\hat{\Omega}<0} \mathbf{d\Omega}\,\left|\hat{\mathbf{n}}\cdot\hat{\Omega}\right| \boldsymbol{\psi}^{\dagger}(\vec{\mathbf{r}},\mathbf{E},\Omega)\tilde{\boldsymbol{\psi}}(\vec{\mathbf{r}},\mathbf{E},\Omega), \tag{3}$$

where $\tilde{\boldsymbol{\psi}}(\vec{\mathbf{r}},\mathbf{E},\Omega)$ is the incoming angular flux (beam) at the boundary [5]. Note that the use of Eqs. (1) and (2) requires modification of the standard MCNP5 weight-window algorithm.

2.1.3. 1D importance function calculation using CEPXS/ONELD

To generate the required importance functions, ADEIS utilizes the CEPXS/ONELD package [4]. A set of processing codes were developed and integrated as part of a simulation sequence using a universal driver (UDR) to manage the simulation. ONELD calculates the importance associated with each phase-space element by solving the one-dimensional adjoint linear Boltzmann equation (ALBE), Eq. 4, using the S_N method.

$$\begin{aligned} &-\mu\frac{\partial}{\partial x}\psi^{\dagger}(x,E,\mu) + \sigma_t(x,E)\,\psi^{\dagger}(x,E,\mu) = \\ &+\int_{4\pi} d\Omega' \int_{0}^{\infty} dE'\sigma_s(x,E\rightarrow E',\mu_0)\,\psi^{\dagger}(\vec{r},E',\mu') + S^{\dagger}(x,E,\mu) \end{aligned} \tag{4}$$

For electrons, however, the use of the ALBE with the standard Legendre expansion of the scattering kernel is impractical. This can be explained by the fact that unreasonably high expansion order is needed because of the highly anisotropic behavior of the electron scattering process. In order to improve the efficiency of the electron transport calculation, CEPXS generates *effective* cross sections by using the following treatments:

i) A continuous slowing-down (CSD) [6] approximation is used for electron inelastic scattering interactions resulting in small-energy changes (often referred to as soft collisions).

ii) The extended transport correction [7] is applied to the forward-peaked elastic scattering cross-section.

Due to the numerical difficulties inherent to deterministic electron-photon-positron transport calculations, the importance functions may exhibit unphysical oscillations. Moreover, CEPXS/ONELD methodology can produce negative importance functions which cannot be used

to calculate physical quantities such as the lower-weight bounds. Therefore, ADEIS eliminates these undesirable characteristics by a proper selection of the spatial meshing and a simple smoothing procedure. Previous studies using the ADEIS [1, 8] methodology have shown that such approximated importance functions still result in significant increase in the figure-of-merit (FOM, see Eq. 5).

Note that using CEPXS/ONELD is suitable because, at this point, ADEIS uses 1D importance functions to bias the transport process. This implies that the geometries considered must be highly one-dimensional in nature for these importance functions to be accurate enough for transport biasing.

2.1.4. Automatic spatial meshing

It was shown in earlier studies [1, 4] that improper meshing can introduce unphysical oscillations in the importance function and increase statistical fluctuations in the photon tallies. Moreover, determining a spatial mesh structure for a given problem is time consuming and therefore, it was decided to automate the generation of the deterministic model from the MCNP5 combinatorial geometry description. To achieve that goal, material discontinuities are first detected along the "line of sight" and represented as coarse mesh boundaries.

Preliminary studies indicate that a near optimum meshing can be obtain by defining the deterministic (and associated weight-window) mesh size to about half of an average condensed history (CH) step size. This ensures that on average every weight-window event occurs in a different mesh. Moreover, this criterion also follows the approximate rule-of-thumb [4],

$$\frac{\upsilon \times R(E_1)}{G} < \Delta x < 0.1 \times R(E_1) \tag{5}$$

where $R(E_1)$ is the range associated with electron in the fastest energy group, G is the total number of groups and ν is the ratio of the mean vector range to the CSD range. This rule ensures that possible fluctuations in the "energy domain" are not transmitted to the "spatial domain" by maintaining a mesh size larger than the partial range associated with the slowing down of electrons from one group to the next.

2.1.5. Positron biasing

In MCNP5, the traditional approach is to transport the electrons and positrons using the same physical models and only "flag" the particle as a positron for special purposes such as annihilation photon creation and charge deposition. However, due to the possibility of creating relatively high energy photons from low energy positrons, the importance function of positrons can be significantly different from the importance function of electrons as illustrated in Fig. 3, which shows the ratio of electron to positron importance functions.

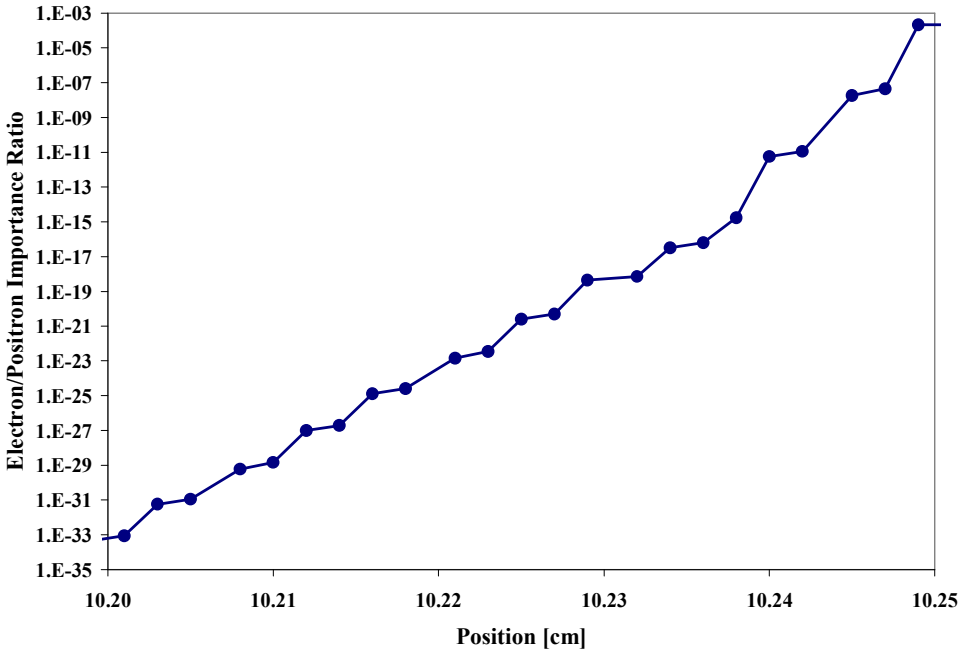

Figure 3 Ratio of Electron to Photon Importance Functions in the Flattening Filter

Therefore, in ADEIS, it is possible to generate lower-weight bounds for positrons that are different than the lower-weight bounds for electrons. The standard MCNP5 weight-window was modified to explicitly bias the positrons using the appropriate lower-weight bounds.

2.2. Performance of an MC simulation

When evaluating the efficiency of any non-analog MC simulation, three factors are important, i) the history scoring efficiency, ii) the dispersion of non-zero scores, and iii) the computer time per history. The first factor is essentially the fraction of source particles that contribute to a given tally, the second factor is related to the spread of the particle weights scoring and therefore the variance of a tally and the third is related to the number of histories that can be simulated in a given unit of time. Therefore, the scoring efficiency, the ratio of the largest tally score to the average tally score and the number of simulated history per minute can be used to take a detailed look at the performance of the simulation. Moreover, these three factors are generally folded into a single metric to get a figure-of-merit (FOM) describing the performance of the simulation. This FOM is evaluated according to the following formulation,

$$FOM = \frac{1}{R^2 T} \tag{6}$$

which can also be used to evaluate the overall performance of a simulation.

3. TEST PROBLEMS

For all the analyses presented in this paper, we are considering a mono-energetic 6 MeV electron beam impinging on a tungsten target producing bremsstrahlung photons, which are transported through a heterogeneous material distribution representing a simplified accelerator head and patient as shown in Fig. 4.

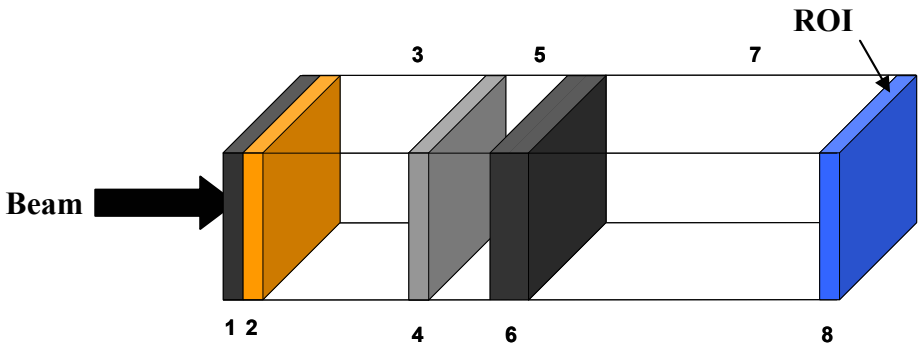

Figure 4 Test Problem Geometry

For these studies, the objective is to obtain the photon total fluxes as well as the spectra in the region of interest (ROI) which is colored in blue in Fig. 4 (region 8, located on the right side of the model). This region is a layer of water representing the patient is located at 100 cm away from the source. The details associated with each zone of Fig. 4 are presented in Table I.

Table I. Geometry Description for Reference Case

Zone	Description	Color	Material	Size (cm)
1	Target	Dark Gray	Tungsten	0.1
2	Heat Dissipator	Orange	Copper	0.15
3	Vacuum	White	Low Density Air	8.75
4	Vacuum Window	Light Gray	Beryllium	0.05
5	Air	White	Air	1.1
6	Flattening Filter	Dark Gray	Tungsten	0.1
7	Air	White	Air	88.85
8	Region of Interest	Blue	Water	10

Table II shows the various Monte Carlo and deterministic parameters used throughout this work.

Table II. Reference Simulation Parameters

Determinisic (ONELD)	Monte Carlo (MCNP5)
Flat adjoint source spectrum in electron groups only	6 MeV monodirectional electrons
50 electron groups 42 photon groups (log structure)	Electrons and photons
S_{16}-P_{15}	Default values of step size
Detailed physics including energy straggling	Detailed physics including energy straggling
0.001 MeV cutoff	0.001 MeV cutoff

4. POSITRON BIASING

To address the issue of importance quality and positron biasing, this section presents results from simulation of the test problem using the standard MCNP5, ADEIS without explicit positron biasing and ADEIS with explicit positron biasing.

4.1. "Real" positron importance function

In previous work [1], we showed that the large discontinuity in importance function between electron/positron and photon at a given location can produce statistical fluctuations under certain conditions. Table III shows the ratio of photon to electron/positron importance at the interface between regions 6 and 7 (in Fig. 4) for the fastest energy group.

Table III. Ratio of Electron/Positron to Photon Importance

Electron/positron Importance	2.106E-05
Photon Importance	0.637
Ratio	3.31E-05

It was shown that such a ratio ($\sim 10^{-5}$) between the importance functions produces statistical fluctuations in the photon tallies. This is due to positrons surviving Russian roulette games and having their weight increased significantly due to the low importance predicted by the electron/positron lower-weight bounds. Consequently, annihilation photons generated by this positron can produce infrequent high weight scores in the tally, therefore leading to statistical fluctuations.

However this effect is “artificial”, since when comparing the photon importance function to the explicit positron importance function at this location this ratio is greatly reduced. Table IV presents the “real” ratio between positron and photon importance functions at the interface between regions 6 and 7.

Table IV. Ratio of Positron to Photon Importance at the Interface Between Regions 6 and 7

Positron Importance	0.1002
Photon Importance	0.637
Ratio	0.157

It is interesting to note that the positron importance is relatively similar to the photon importance, and at low energies, even becomes larger. It is also interesting to compare the photon and positron importance functions throughout the model as shown in Fig. 5.

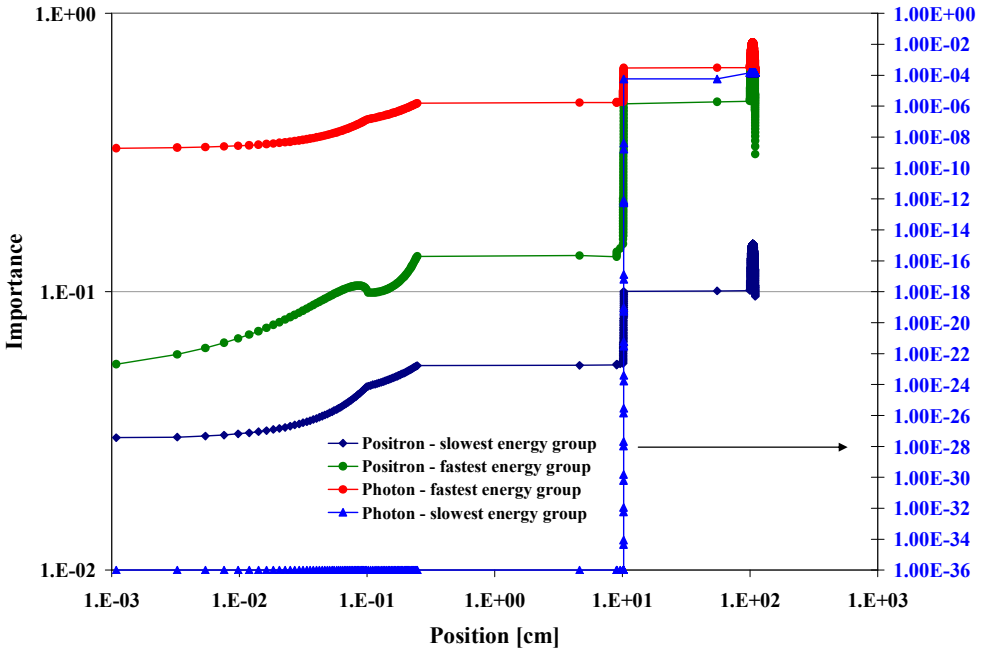

Figure 5 Photon and Positron Importance throughout Test Problem

Fig. 5 shows that the positron importance function closely resembles the photon importance function. This suggests that for certain specific problems, it may be possible to replace the “electron/positron” lower-weight in the standard MCNP5 by the photon lower-weight and therefore in the process mitigate the fluctuations caused by using the electron importance function.

Clearly the use of electron importance functions to bias positrons results in "too many" roulette events and this excessive rouletting of positrons produces an undersampling of the annihilation photons. The undersampling of the annihilation photons can be seen in Table V, which compares the average weight per source particle created through annihilation photon for the standard MCNP5 simulation as well as for ADEIS with and without explicit positron biasing.

Table V. Impact of Positron Biasing

Case	Annihilation Photon Weight / Source Particle
Standard MCNP5	1.646E-02
ADEIS	3.51E-04
ADEIS with positron biasing	1.652E-02

Table V indicates that the annihilation photons are undersampled in the case where ADEIS does not includes explicit positron biasing.

4.2. Photon flux energy spectrum

It is important to examine the energy spectrum of the photons in the ROI. Fig. 6 shows the average photon flux spectrum in the ROI. Note that in Fig. 6, the average 1-σ statistical uncertainty is less the 1% and error bars are about the size of the symbols used.

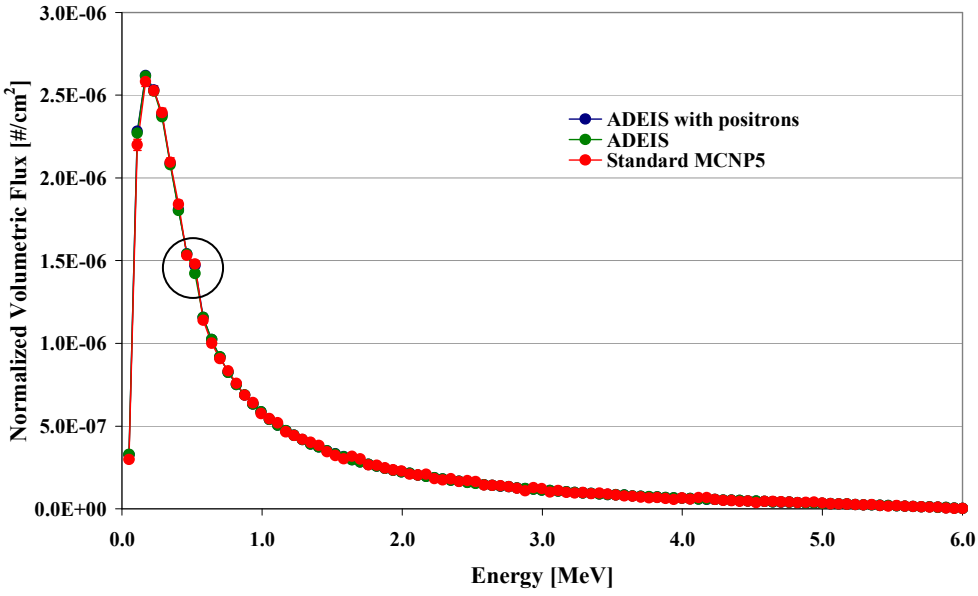

Figure 6 Average Photon Flux Spectra in Region-of-Interest (ROI)

Fig. 6 shows that the spectra obtained with each method are within statistical uncertainties except at one energy bin. The segment of the spectrum that contains that energy bin is shown in Fig. 7.

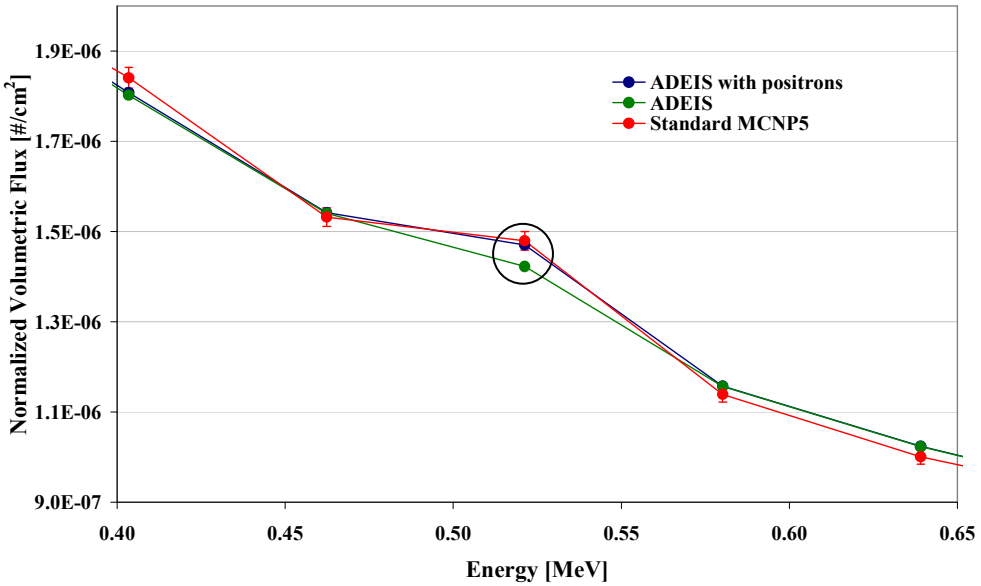

Figure 7 Photon Flux Spectrum Segment with Biased Energy Bin

Fig. 7 shows that when the positrons are not biased explicitly, the single energy bin presenting a bias slightly larger (~ 4%) than the statistical uncertainty. This effect can be attributed to the annihilation photons, because the energy range of that bin is 0.5 MeV to 0.525 MeV.

It is also interesting to examine the surface photon flux spectrum at the interface between regions 6 and 7. By examining the spectrum coming out of that region, it is possible to better observe the impact of the positron biasing through the annihilation photons before this effect is "smeared" by scattering. The surface photon flux spectra at the interface between the two regions are shown in Fig. 8.

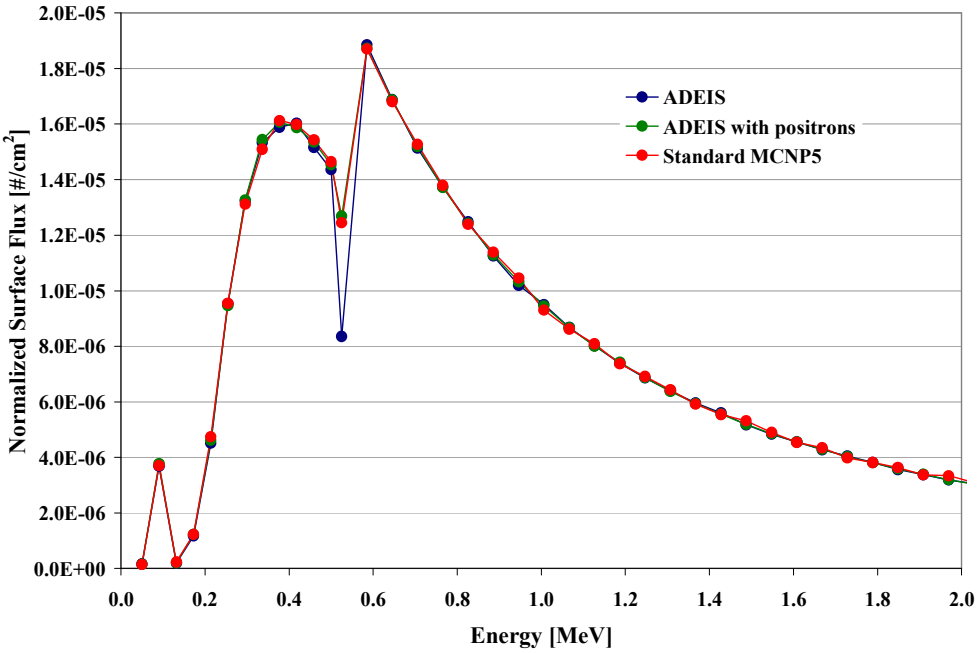

Figure 8 Surface Photon Flux Spectra at Tungsten-Air Interface

Fig. 8 shows clearly the undersampling of the annihilation photons which can be attributed to excess amount of rouletting performed by ADEIS when positrons are biased using the electron importance function. Note that the 1-σ statistical uncertainty is below 1% and the error bars are smaller then symbols used.

4.3. Speedup & performance

The speedup obtained from the ADEIS can be estimated by calculating the ratio of the FOM for the different VR cases with the standard MCNP5. Table VI shows that, for this problem, ADEIS results in a speedup of ~14.

Table VI. FOM and Speedup for Photon Tallies

Case	FOM (speedup)
Standard MCNP5	25
ADEIS	235 (9.4)
ADEIS with positron biasing	360 (14.4)

It worth noting that, as shown in previous work [1, 8], higher speedups are expected as the probability of transmission from the source to the ROI decreases.

5. SUMMARY & CONCLUSIONS

In this work, it was shown that the importance quality can significantly affect the efficiency and/or the accuracy of variance reduction technique using splitting/rouletting in coupled electron-photon-positron simulations. More specifically, it was shown that not explicitly biasing the positrons with their own set of importance functions results in an undersampling of the annihilation photons and consequently, introduces a bias in the results.

It is important to note that the computational cost (upscattering) of generating coupled electron-photon-positron importance functions may become noticeable in multidimensional problems, therefore ADEIS includes the necessary logic is included to prevents explicit simulation of positrons if the photons energy is less than 1.022 MeV. Our future work will address the determination and use of multi-dimensional importance functions.

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