Approximating Secondary Photon Generation for the Deterministic Photon Transport Calculations

Nhan Nguyen Trong Mai [a], Kyeongwon Kim [a], Deokjung Lee [a*]
[a] *Department of Nuclear Engineering, Ulsan National Institute of Science and Technology, 50 UNIST-gil, Ulsan 44919, Republic of Korea*
[*] *Corresponding author: deokjung@unist.ac.kr*

1. Introduction

Photon transport is becoming prevalent in the high-fidelity nuclear reactor analysis. However, the secondary photon generated from atomic relaxation and Bremsstrahlung process [1] are often neglected in the deterministic photon transport calculation to reduce the complexity. The energy of secondary photon is assumed to be deposited locally with this approach [2]. Although the lack of secondary photon transport does not introduce significant error to photon heating calculation for Light Water Reactor (LWR) problems, it does notably affect the photon spectrum from few keV to several MeV [3].

The incorporation of the secondary photon source will yield a more accurate photon spectrum, which will be valuable for further applications such as gamma detector calculation. This paper presents the approximation utilized to compute the secondary photon source.

2. Methods

The multigroup production cross-section (XS) for secondary particles generated from photon interactions are presented in section 2.1 and 2.2. The bremsstrahlung approximation is given in section 2.3.

2.1 Photoelectric

Each photoelectric event produces one photoelectron (*pe*) whose spectrum is described as:

$$F_{pe}^{ie}(E,ssi)=\begin{cases}1, & \left(E-EB_{ssi}\right)\in ie\\ 0, & \left(E-EB_{ssi}\right)\notin ie\end{cases} \tag{1}$$

where ie is the index of electron group, E is the incident photon energy, ssi is the electron shell that emit the photoelectron, EB_{ssi} is the binding energy of electron shell ssi.

The multigroup production XS for photoelectron is computed by:

$$\sigma_{pe}^{ip\to ie}=\frac{\sum_{ssi=1}^{TNS}\left[\int_{ip}F_{pe}^{ie}\left(E,ssi\right)\sigma_{ss}\left(E,ssi\right)\phi_p\left(E\right)dE\right]}{\int_{ip}\phi_p\left(E\right)dE} \tag{2}$$

where ip is the index of photon group, TNS is the total number of electron subshells, $\sigma_{ss}\left(E,ssi\right)$ is the photoelectric XS of subshell ssi, and $\phi_p\left(E\right)$ is the photon flux weighting function.

Because the combination of electron subshells for possible transitions in atomic relaxation is tremendous [1]. The spectrum of fluorescence photons (*fl*) and Auger electrons (*Ae*) following the ejection of the photoelectron is computed by Monte Carlo method instead of the derivation of mathematic models. The cumulative density function (CDF) for sampling process is based on the available transition probabilities of fluorescence photon/Auger electron.

A vacancy queue is initialized for subshell ssi and the following steps are employed:

a) Take one vacancy in the queue.
b) Sample transition according to CDF. If no electron is left on this subshell, repeat this step.
c) If a fluorescence photon is sampled by transition from shell ssj : $F_{fl}^{ip}(ssi)=F_{fl}^{ip}(ssi)+1$, add one new vacancy at ssj to the vacancy queue.
d) If a Auger electron is sampled by transition from ssj : $F_{Ae}^{ie}(ssi)=F_{Ae}^{ie}(ssi)+1$, add one new vacancy at ssj and one new vacancy at ssk to the vacancy queue (ssk is where Auger electron emitted)
e) Go back to step a) until no vacancies are left.

The multigroup production XS for fluorescence photon is computed by:

$$\sigma_{fl}^{ip\to ip'}=\frac{\sum_{ssi=1}^{TNS}\left[\int_{ip}F_{fl}^{ip'}\left(ssi\right)\sigma_{ss}\left(E,ssi\right)\phi_p\left(E\right)dE\right]}{\int_{ip}\phi_p\left(E\right)dE} \tag{3}$$

The multigroup production XS for Auger electron $\sigma_{Ae}^{ip\to ie}$ is computed by replacing $F_{fl}^{ip'}\left(ssi\right)$ with $F_{Ae}^{ie}\left(ssi\right)$ in Equation (3).

It is noted that the photon flux weighting is pre-generated and represents a typical photon spectrum of the considered problems.

2.2 Compton scattering and pair production

The differential cross-sections (DCS) commonly used in Monte Carlo codes to sample the outgoing energy of charged particles, namely the Klein-Nishina DCS for electron in Compton scattering (*Com*) and the Davies-Bethe-Maximon DCS for electrons and positrons from pair production (*pp*) [4-7], are used to compute the emission spectrum of electron from Compton scattering (*Ce*) and positron (*po*) from pair production:

$$F_{Ce/po}^{ie}(E) = \frac{\int_{ie} \left(\frac{d\sigma}{dT}\right)_{Com/pp} dT}{\int_{T_{\min}}^{T_{\max}} \left(\frac{d\sigma}{dT}\right)_{Com/pp} dT} \tag{4}$$

where $\frac{d\sigma}{dT}$ is the DCS as a function of the energy of the charged particles T.

The multigroup production XS for electron from Compton scattering is:

$$\sigma_{Ce}^{ip\rightarrow ie} = \frac{\int_{ip} F_{Ce}^{ie}(E)\sigma_{Com}(E)\phi_p(E)dE}{\int_{ip} \phi_p(E)dE} \tag{5}$$

where σ_{Com} is the Compton XS.

The multigroup production XS for positron is obtained in a similar fashion:

$$\sigma_{po}^{ip\rightarrow ie} = \frac{\int_{ip} F_{po}^{ie}(E)\sigma_{pp}(E)\phi_p(E)dE}{\int_{ip} \phi_p(E)dE} \tag{6}$$

where σ_{pp} is the pair production XS. It is noted that electrons from pair production have the same production XS as positrons due to the nature of the Davies-Bethe-Maximon DCS [7].

The fluorescence photon sources, electron sources or positron sources are simply computed by the convolution of the photon flux with the respected production XS.

2.3 Bremsstrahlung

The electron and positron source are subject to the slowing down process and bremsstrahlung photon will be emitted as a result. The charged particles will not be transported, and the following approximation is used:

- the emission of photon is isotropic.
- the continuous-slowing down approximation is employed, where the charged particles lose their energy continuously at a rate determined by the stopping power [8]

The number of photons emitted with energy higher than E_{cut} induced by an electron with initial energy T is:

$$Y(T, E_{cut}) = \int_{E_{cut}}^{T} \frac{\Sigma_{br}(T', E_{cut})}{S_{tot}(T')} dT' \tag{7}$$

where $\Sigma_{br}(T, E_{cut})$ is the bremsstrahlung XS, and $S_{tot}(T)$ is the total stopping power [6,7]. The emission spectrum for photon in group ip (E_1 to E_2) by electron T is [9]:

$$F_{br}^{ip}(T) = Y(T, E_2) - Y(T, E_1) \tag{8}$$

The total number of bremsstrahlung photon emitted by electron in group ie is:

$$C_{el}^{ie\rightarrow ip} = \frac{\int_{ie} F_{br}^{ip}(T) w_e(T) dT}{\int_{ie} w_e(T) dT} \tag{9}$$

where $w_e(T)$ is a weighting function for electron.

The bremsstrahlung photon emitted by electron is obtained by the convolution of this factor $C_{el}^{ie\rightarrow ip}$ with the electron source. A similar approach is applied for photon emitted from the slowing down of positions.

3. Verification

STREAM is a specialized deterministic code developed by the Computational Reactor Physics and Experiment laboratory (CORE) of the Ulsan National Institute of Science and Technology (UNIST) for the analysis of LWR problems [10]. STREAM uses the method of characteristic to solve the neutron transport equation. The implemented photon module in STREAM did not consider secondary photons [3]. Thus, the above-mentioned approximations are incorporated into the existing photon module in STREAM with the following adaptations:

- The fluorescence photon is treated as $(\gamma, n\gamma')$ scattering $(n \geq 1)$ and the fluorescence photon production XS is added directly into the scattering matrix.
- the positron annihilation is also treated as $(\gamma, 2\gamma')$ scattering.
- The bremsstrahlung sources are computed based on the charged particle sources. The total photon source now consists of the neutron-induced

photon sources, the scattering photon sources (with fluorescence), and the bremsstrahlung photon sources.

- The photon fixed-source solver is conducted with this combined photon sources.

It is noted that all the prevalent photon data employed in this approximation, namely transition energies, binding energies, the number of electrons in subshells, transition probabilities are obtained from the EPICS2014 library [11]. The photo atomic XS is obtained from the ENDF/B-VII. 1 nuclear data [12].

The Monte Carlo code MCS also developed at UNIST [13] is used for the verification because atomic relaxation and bremsstrahlung models are viable [6]. MCS is also used to generate the weighting photon flux $\phi_p(E)$ by tallying the photon flux in a LWR pin cell using thousand energy bins. Billion histories are used to achieve the relative error less than 1% for most of the bins.

The VERA 1B pin cell problem [14] is selected, and the photon flux obtained with STREAM in different material regions is compared to those obtained from MCS. The configuration of the tested problem is given in Figure 1.

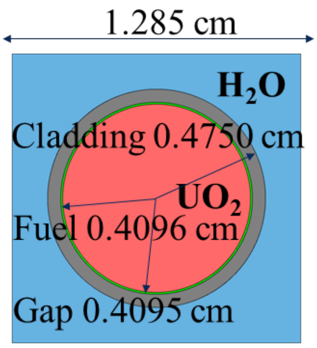

Figure 1. VERA 1B pin cell.

The photon flux comparison with MCS is given in Figure 2. The calculation that incorporates the secondary photon source is denoted as *ST(ArBr)* whereas *ST(default)* indicates calculation that neglect the secondary photons.

The photon flux from *ST(ArBr)* exhibits significant improvement in comparison to *ST(default)*. Specifically, the photon flux above 200 keV closely aligns with MCS results. The discrepancies below 200keV for *ST(default)* is largely attributed to the lack of atomic relaxation.

ST(ArBr), a combination of *ST(default)* and the incorporation of secondary photon transport, naturally inherits some distinctions from *ST(default)* in this energy range. While the observed differences in *ST(ArBr)* below 200 keV are inevitable due to *ST(default)*'s inherent disparities, they remain quite minimal. Furthermore, photon flux within this range is considerably lower, ranging from ten to a hundred times, compared to flux levels at several MeV.

4. Conclusions

In conclusion, the presented method offers an effective means to integrate secondary photon sources into deterministic photon transport calculations. By computing fluorescence photons and charged particle sources through the multigroup production XS and applying the continuous slowing down approximation for bremsstrahlung photon sources, the resulting photon spectra exhibit improved accuracy. Verification against MCS results validates the approach, highlighting the enhanced photon flux computed by STREAM.

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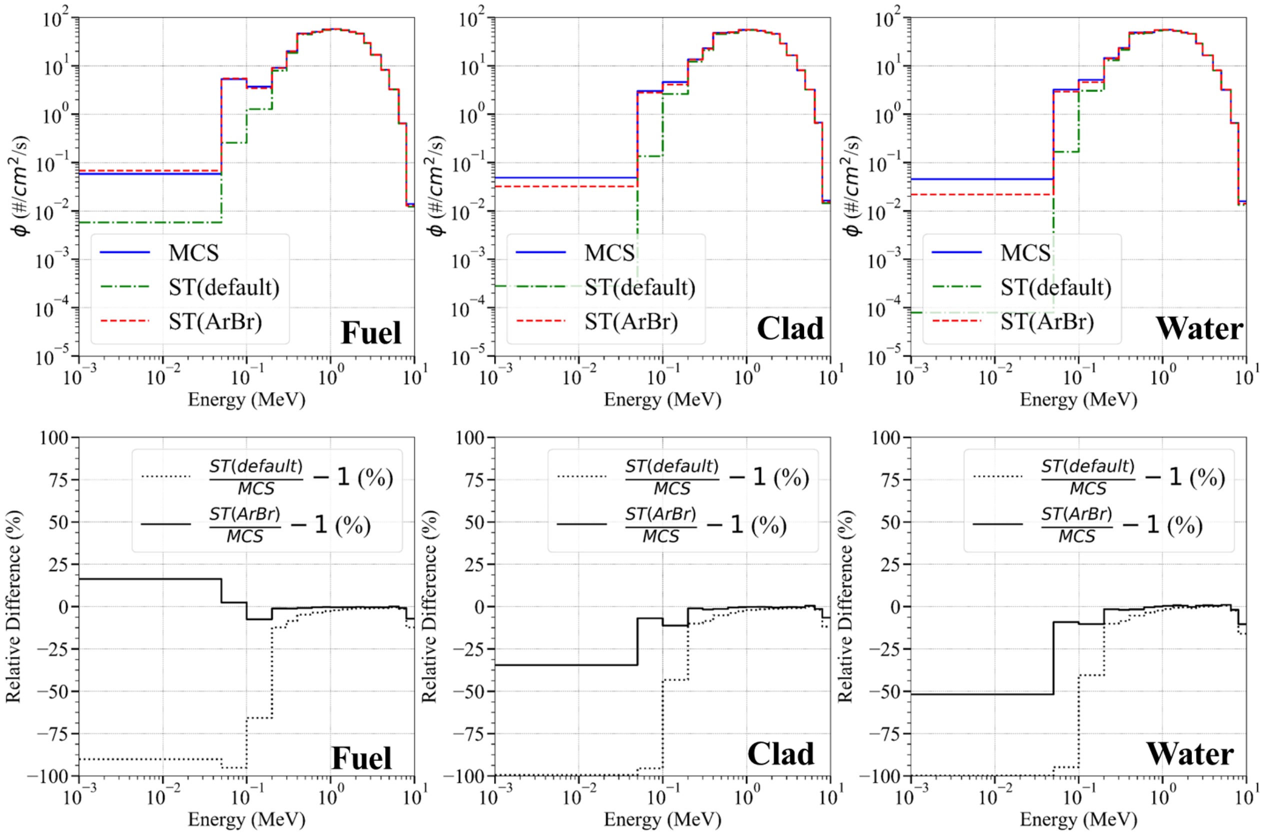

Figure 2. Comparison of photon flux with MCS