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FAST GAMMA RAY LEAKAGE SPECTRA SIMULATION

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ABSTRACT

We present the simulation of the decay gamma source leakage spectra. In order to solve this problem we are developing the SGRD code (Spectroscopy, Gamma-ray, Rapid, and Deterministic). The main goal of this software is to perform fast and accurate 1D spherical calculation. For this purpose, the collided and uncollided parts of the flux spectrum are calculated separately using the discrete ordinates S_N method. The uncollided part is calculated by transporting each source line and the collided component is computed using the multigroup method. Comparison of gamma leakage spectra with a reference MCNP5 calculation on a typical test problem shows that accurate results are obtained and the computational time is several orders of magnitude shorter with SGRD.

Key Words: Gamma-Ray Spectroscopy, Deterministic Transport, Computer Code

1. INTRODUCTION

Regarding nuclear safeguards, gamma-ray spectroscopy [1] is one of the most prominent methods used for isotopic assay of Special Nuclear Material (SNM). The gamma line structure is a unique signature of a given isotope composition and gamma line intensity is proportional to the number of atoms in a measured sample.

For real-time analysis and iterative inversion problems, the computational time is a very important issue. For that purpose we are developing the SGRD code (Spectroscopy, Gamma-ray, Rapid, and Deterministic) which uses the multigroup, one dimensional, spherical discrete ordinates solver of PANDA transport library [2]. Deterministic methods are used in rapid gamma ray spectra simulation tools [3,4] because, for simple models they have a higher computational time efficiency than Monte-Carlo methods.

The multigroup method is used only for computation of the collided part of the spectrum; on the other hand, the discrete direct spectrum is calculated by transporting each γ source line. The discrete source term is calculated using DARWIN [5] code.

In the first part we describe the simulation of the decay gamma source leakage spectra with SGRD software. In a second part we present a test problem with comparisons between SGRD and MCNP5 [6] results.

2. METHODS

2.1. Problem Geometry and Sources

The problem is to determine the gamma-ray leakage at the external boundary of a one-dimensional spherical assembly. The assembly is composed of concentric shells. Each shell is characterized by its atomic composition and density and can be associated with a gamma source term.

The gamma-ray source is composed of discrete lines emitted by the unstable isotopes. A typical source term can be composed of more than a thousand discrete gamma lines.

2.2. Treatment of the energy variable

The gamma flux produced by the source lines is obtained by solving the Boltzmann equation using the multigroup discrete ordinates method [7]. The energy variable range is divided into *G* groups and the gamma flux is solution of a set of *G* coupled multigroup equations.

The computational efficiency of the method is highly dependent on the group number. Therefore, a straightforward application of the multigroup method is not optimal in term of computational time because a great number of energy groups are necessary to accommodate the thin gamma lines.

One can notice that the flux spectrum is made of two distinct components, the collided or scattered one and the uncollided or direct one. The uncollided component is a discrete set of thin lines and the collided component is a smooth scattered background. This remark leads us to use the multigroup method only for the scattered component of the flux because it requires only a moderate number of groups (about one hundred).

The flux computation is performed using three transport calculations.

- The first step is the uncollided transport of each source line;

$$\vec{\Omega}\cdot\vec{\nabla}\varphi^{UNC}\left(E_\gamma\right)+\sigma_T\left(E_\gamma\right)\varphi^{UNC}\left(E_\gamma\right)=q\left(E_\gamma\right) \tag{1}$$

- The second step is the total multigroup transport with the collision term of the multigroup source. The multigroup source is obtained by condensing the gamma lines into groups ($q\left(E_\gamma\right)\rightarrow q_g$).

$$\vec{\Omega}\cdot\vec{\nabla}\varphi_g^{TOT}+\sigma_g^T\varphi_g^{TOT}=\sum_{g'=1}^{G}\int_{4\pi}\sigma_{g'g}\left(\vec{\Omega}'\cdot\vec{\Omega}\right)\varphi_{g'}^{TOT}\left(\vec{\Omega}'\right)d\Omega'+q_g \tag{2}$$

- The third step is the uncollided transport of the multigroup source.

$$\vec{\Omega}\cdot\vec{\nabla}\varphi_g^{UNC}+\sigma_g^T\varphi_g^{UNC}=q_g \tag{3}$$

The scattered component is given by subtracting the uncollided multigroup flux to the total multigroup flux.

$$\varphi_g^{COL}=\varphi_g^{TOT}-\varphi_g^{UNC} \tag{4}$$

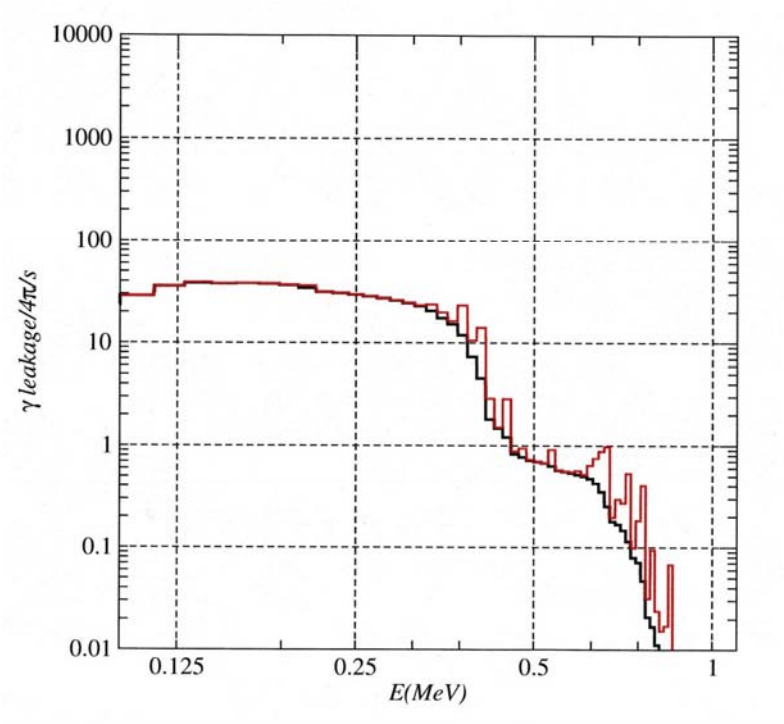

Figure 1. Example of total (collided plus uncollided) multigroup γ leakage spectra (red) and collided only component (black)

The outward leakage spectrum *F* is calculated using the angular flux at the external boundary.

$$F^{UNC}\left(E_\gamma\right)=4\pi R^2\left(\frac{1}{2}\int_0^1\varphi^{UNC}\left(E_\gamma,R,\mu\right)\mu d\mu\right) \tag{5}$$

$$F_g^{COL}=4\pi R^2\left(\frac{1}{2}\int_0^1\varphi_g^{COL}\left(R,\mu\right)\mu d\mu\right) \tag{6}$$

The total leakage spectrum is the superposition of the discrete uncollided and multigroup scattered components on a very fine multigroup uniform grid (typical channel width ΔE_γ=0.25 keV).

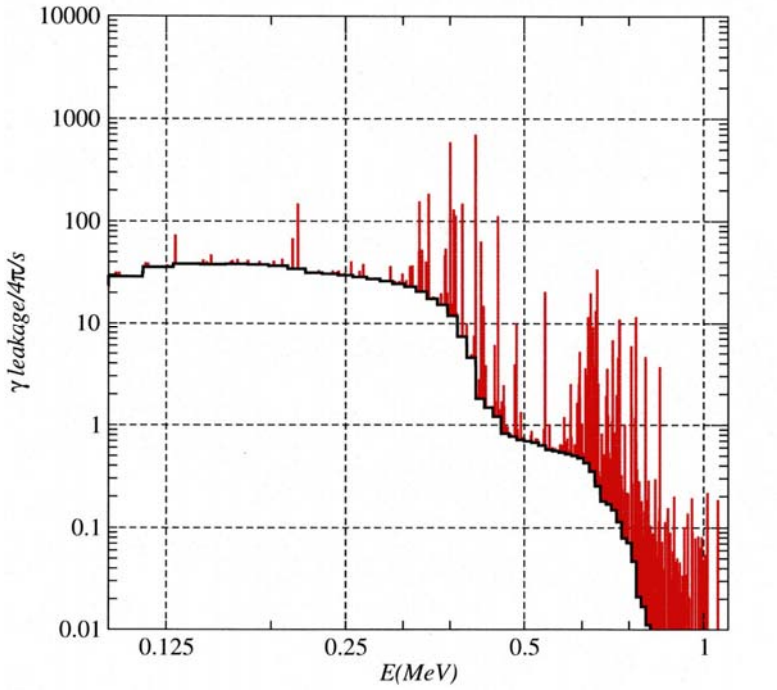

Figure 2. Example of SGRD calculated spectra with multigroup scattered background and point-wise gamma lines.

2.3. Computer Codes

The source term is separately calculated using DARWIN, an isotopic composition evolution code which solves the Bateman equations using JEFF-3.1 radioactive decay data library [8].

For each material, the macroscopic point wise total cross-sections $\sigma_T\left(E_\gamma\right)$, the multigroup total cross-sections σ_g^T and the coefficient of the Legendre polynomial expansion of the group to group scattering cross-section matrix $\sigma^l_{g\to g'}$ are produced by a general purpose, internal cross-section processor code using ENDF/B-VII photo-atomic sublibrary [9].

The transport calculations are performed within the SGRD code which solves the one-dimensional spherical Boltzmann equation using the multigroup discrete-ordinates S_N solver, with anisotropic scattering, of the PANDA neutron transport library. Problem set-up, transport calculations and projection on the broad and fine multigroup grids are performed by the SGRD code.

On a conventional Pentium PC platform, the computation time is a few seconds for a thousand line gamma source problem.

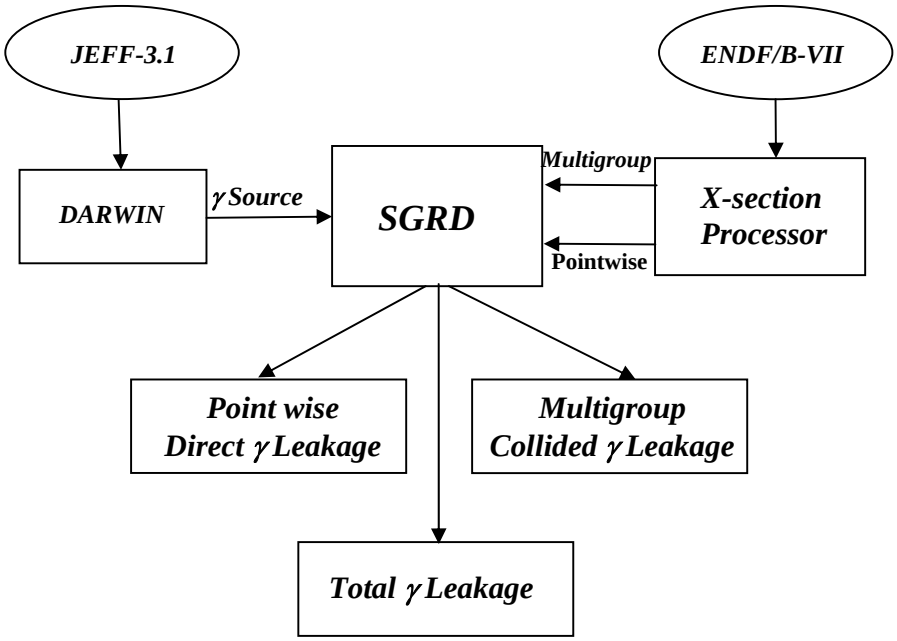

Figure 3. SGRD input/output flow diagram.

3. RESULTS

SGRD software is validated by comparison with MCNP5 calculations. In the presented test problem one consider the gamma leakage spectra of a water reflected sphere of plutonium nitrate solution. This problem is based on a sub-critical version of the PU-SOL-THERM-001 ICSBEP benchmark [10] with a reduced size.

The 1-D Spherical benchmark is composed by an internal sphere of Pu nitrate solution (radius=6.2 cm) contained in a steel shell (1 mm) surrounded by water (40 cm) with an external steel shell (1 cm).

The calculated gamma leakage spectra are presented on figure 4. The two calculations are in good agreement. One can notice that the deterministic calculation of the scattered background is free from statistical noise. The main interest is that the SGRD computation time is of about 1s compared to hours for the Monte Carlo calculation on a typical personal computer.

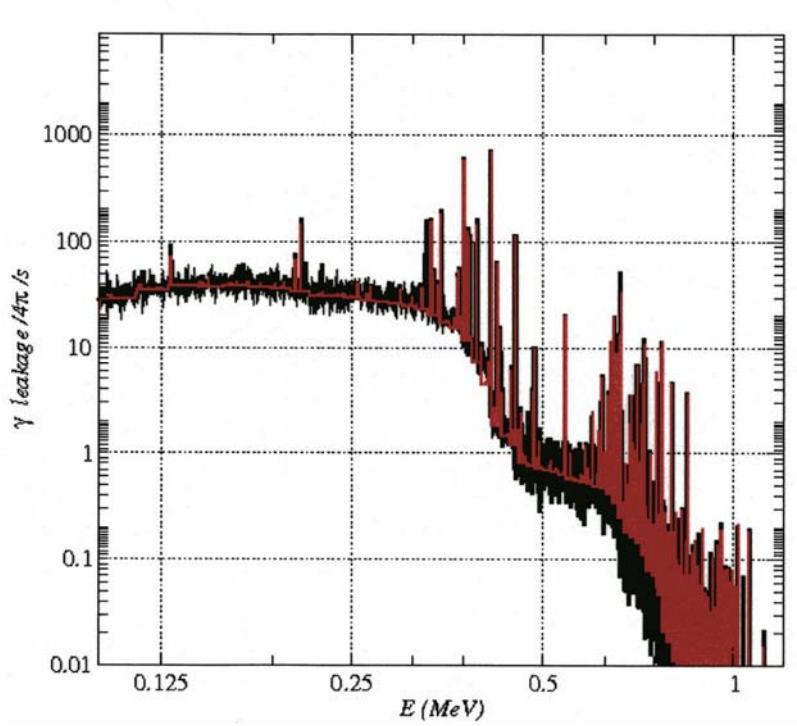

Figure 4. Comparison of SGRD (red) and MCNP5 (black) calculated spectra for the water reflected sphere of plutonium nitrate solution test problem.

3. CONCLUSIONS

The SGRD software has been developed for rapid gamma spectroscopy calculation using 1D spherical modeling with a discrete ordinates multigroup transport solver. In order to improve the computation efficiency, the scattered background and the uncollided gamma lines are separately transported.

Comparison of gamma leakage spectra with a reference MCNP5 calculation on a typical test problem shows that accurate results are obtained and the computational time is several orders of magnitude shorter with SGRD.

In future work, we will take into account the other gamma source terms (bremsstrahlung, (n,γ), spontaneous and induced fission) and the response of gamma-ray spectrometers for comparison with experimental data.

REFERENCES

1. G.F. Knoll, “Radiation Detection and Measurements”, John Wiley and Sons (1999).
2. P. Humbert, “Results for the C5G7 3-D Extension Benchmark Using the Discrete Ordinates Code Panda”, *Progress in Nuclear Energy*, **48**, pp 394-400 (2006).

3. L.E. Smith et al. ,“Deterministic Transport Methods for the Simulation of Gamma-Ray Spectroscopy Scenarios“, Nuclear Symposium Conference Record, 2006 IEEE, Volume **1**, Issue oct. 29, pp 588-592 (2006).
4. D.J. Mitchell, J. Mattingly, “Rapid Computation of Gamma-ray Spectra for One-Dimensional Source Models”, *Trans. Am. Nuc. Soc.*, **98**, pp 565-568 (2008).
5. A. Tsilanizara et al., “DARWIN: an evolution code system for a large range of applications,” Proc. of the 9th Int. Conf. on Radiation Shielding, Tsukuba, Japan, Oct. 17-22, p. 845 (1999).
6. X-5 Monte Carlo Team 2003, MCNP - A General Monte Carlo N-Particle Transport Code Version 5 - Volume I: Overview and Theory (2003).
7. E.E. Lewis and W.F. Miller, “Computational Methods of Neutron Transport”, American Nuclear Society, La Grange Park, IL, (1993).
8. JEFF Report 21, “The JEFF-3.1 Nuclear Data Library”, OECD/NEA No. 6190 (2006).
9. M.B. Chadwick et al., *Nuclear Data Sheets*, **107**, 2931 (2006)
10. R.D. Carter et al., “Water Reflected 11.5 inch Diameter Spheres of Plutonium Nitrate Solutions”, PU-SOL-THERM-01, International Handbook of Evaluated Criticality Benchmark Experiments, NEA/NSC/DOC(95)03, OECD – Nuclear Energy Agency (Rev. Sept 2007).