

Advances in Monte-Carlo code TRIPOLI-4[®]'s treatment of the electromagnetic cascade

Davide Mancusi*, Alice Bonin*, François-Xavier Hugot* and Fadhel Malouch*

*Den-Service d'études des réacteurs et de mathématiques appliquées (SERMA),
CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France
Email: davide.mancusi@cea.fr

Abstract—TRIPOLI-4[®] is a Monte-Carlo particle-transport code developed at CEA-Saclay (France) that is employed in the domains of nuclear-reactor physics, criticality-safety, shielding/radiation protection and nuclear instrumentation. The goal of this paper is to report on current developments, validation and verification made in TRIPOLI-4 in the electron/positron/photon sector. The new capabilities and improvements concern refinements to the electron transport algorithm, the introduction of a charge-deposition score, the new thick-target bremsstrahlung option, the upgrade of the bremsstrahlung model and the improvement of electron angular straggling at low energy. The importance of each of the developments above is illustrated by comparisons with calculations performed with other codes and with experimental data.

I. INTRODUCTION

An accurate description of the electromagnetic cascade is an essential prerequisite for the simulation of the response of a wide range of particle detectors, including in-core and ex-core instrumentation in nuclear reactors. For such applications, one possible simulation tool is provided by the TRIPOLI-4[®] code [1], a Monte-Carlo particle-transport code developed at CEA-Saclay (France) that is employed in the domains of nuclear-reactor physics, criticality-safety, shielding/radiation protection and nuclear instrumentation. The latest TRIPOLI-4 version (v10) was released in December 2015 and will soon be available to OECD member countries through the NEA Data Bank. This extended abstract reports on some recent developments in TRIPOLI-4 for the simulation of nuclear instrumentation (Section II). Section III compares the predictions of the development version of TRIPOLI-4 with those of TRIPOLI-4 v10 and of other transport codes; additionally, we compare the calculation results against selected experimental data. Conclusions and future plans are discussed in Section IV.

II. DESCRIPTION OF SOME RECENT DEVELOPMENTS

We now proceed to describe some of the new developments in detail.

A. Bremsstrahlung model

The production of bremsstrahlung photons by electrons and positrons in TRIPOLI-4 v10 proceeds according to the specifications of the model described in Berger and Seltzer [2] and summarised in Penelieu [3]. However, the same authors presented a newer model for energy-differential cross sections in Seltzer and Berger [4]. Contrary to the 1970 model, the

new model is essentially based on the interpolation of tabulated values. The table values are derived from numerical phase-shift calculations for electron energies lower than 2 MeV, and from the analytical high-energy theory above 50 MeV; a numerical interpolation scheme was used to cover the intermediate-energy region. Seltzer and Berger's 1986 model may be considered as the state of the art of the field. It is currently implemented in Geant4 [5], [6] and MCNP6 [7].

We introduced Seltzer and Berger's 1986 model and tables as the new default model for bremsstrahlung in the development version of TRIPOLI-4. A new TRIPOLI-4 keyword was added to control the choice of the bremsstrahlung model.

B. Electron angular straggling at low energy

In TRIPOLI-4, electron angular straggling is described by the Goudsmit-Saunderson model [8]. The Goudsmit-Saunderson formalism can in principle be used to condense elastic cross sections from any model/table. In TRIPOLI-4, the cross sections are extracted from different sources depending on the electron energy. Above 256 keV, TRIPOLI-4 uses the Mott cross section [9] with Molière's screening correction [10], [11], as calculated by Feshbach [12] and Sherman [13]. At 256 keV and below, TRIPOLI-4 makes use of data from the Evaluated Electron Data Library (EEDL) [14], which provides integrated and angle-differential large-angle ($\cos \theta < 1 - 10^{-6}$) elastic cross sections. Due to a bug in the processing of the cross sections, angular straggling was overestimated below 256 keV. The correction, which was applied to the development version of the code, results in more forward-peaked angular distributions.

C. Charge-deposition score

Self-powered neutron and gamma detectors (SPND and SPGD), often referred to as *collectrons*, are passive devices for in-core measurement of neutron and/or gamma flux. The basic mechanism underlying collectrons is that matter ionized by neutrons or gammas will in general exhibit some degree of spontaneous electrical polarization, which can be detected using appropriate instrumentation. The resulting current, which is ultimately due to electron and positron transport, increases as the radiation field becomes more intense.

In order to characterize the response of a collectron with a Monte-Carlo simulation, it is necessary to calculate the charge-

deposition distribution in the instrument. This capability was added to TRIPOLI-4 in version 10.

D. Thick-target bremsstrahlung mode

The full simulation of the electromagnetic cascade, including electron and positron transport, is very CPU intensive when compared to a pure photon simulation. However, pure photon transport does not take into account bremsstrahlung photons emitted by secondary electrons; when the photon energy is sufficiently high (say above 1 MeV), pure photon transport will underestimate the secondary photon flux. In cases where a rough estimation of the secondary bremsstrahlung flux is sufficient, it is advantageous to consider a simplified calculation mode (*thick-target bremsstrahlung*, TTB) where electron production and transport are directly replaced by the emission of secondary bremsstrahlung photons; this effectively amounts to replacing secondary electron production with a photon-photon scattering vertex. Since the additional secondary photons are emitted from the starting point of the suppressed electron track, the approximation is generally understood to be less severe in thick volumes, hence its name. A similar approximation exists in MCNP6 [7]. Contrary to TRIPOLI-4, MCNP6's TTB approximation is activated by default in pure photon calculations.

The TRIPOLI-4 TTB implementation proceeds along the lines indicated by Ridoux, Kitsos, Diop, *et al.* [15] and Riz [16]. The most notable difference with respect to the MCNP6 implementation concerns the fact that TRIPOLI-4 accounts for the angular straggling of the condensed electrons; therefore, the bremsstrahlung photons are not necessarily emitted around the initial electron direction. Additionally, the TRIPOLI-4 TTB implementation also allows the use of electron sources; in this case, only tertiary electrons generated by secondary photons are replaced with the corresponding bremsstrahlung photons.

III. VERIFICATION AND VALIDATION

As an example of validation of the new developments for low-energy electrons, we present the comparison of TRIPOLI-4 calculation with an electron transmission/reflection experiment. Seltzer and Berger [17] characterised transmission, reflection and absorption of 100 keV to 400 keV electrons through aluminium and titanium foils of various thicknesses. They report measured values of the number transmission (T_N) and reflection coefficients (R_N), which respectively represent the average number of transmitted (reflected) electrons per incident electron. They also measured energy transmission (T_E) and reflection coefficients (R_E), which respectively represent the fraction of the beam energy that is transmitted through (reflected by) the foil. By difference, one can also define the energy absorption coefficient $\phi_A = 1 - T_E - R_E$. Finally, they also measured the angular distributions of the transmitted electron beams, which however we will not discuss in the present work.

In this work, we limit our comparisons to a subset of the measured data. We concentrate on transmission and reflection

Table I
TRANSMISSION, REFLECTION AND ABSORPTION COEFFICIENTS FOR 100 keV ELECTRONS THROUGH 25.4 μm -THICK ALUMINIUM AND TITANIUM FOILS, EXPRESSED IN PERCENTAGE POINTS. THE MEASURED VALUES ARE TAKEN FROM SELTZER AND BERGER [17]. CALCULATIONS WERE PERFORMED WITH TRIPOLI-4 v10 AND TRIPOLI-4 (DEVELOPMENT VERSION); THE GEANT4 VALUES ARE TAKEN FROM KADRI, IVANCHENKO, GHARBI, *et al.* [18]. THE STATISTICAL UNCERTAINTIES ON THE TRIPOLI-4 VALUES ARE SMALLER THAN THE LAST REPORTED SIGNIFICANT DIGIT. SEE TEXT FOR THE DEFINITION OF THE COEFFICIENTS.

| | exp (%) | TRIPOLI-4 v10 (%) | TRIPOLI-4 dev (%) | Geant4 (%) | |
|----|------------|-------------------------|-------------------------|---------------|------|
| Al | T_N | 60.2 ± 6.0 | 18.2 | 65.4 | 60.7 |
| | R_N | 12.4 ± 0.1 | 64.7 | 9.0 | 12.6 |
| | T_E | 39.3 ± 3.9 | 6.7 | 42.4 | 40.3 |
| | R_E | 7.1 ± 0.7 | 43.2 | 4.5 | 7.2 |
| | ϕ_A | 53.6 ± 5.4 | 50.2 | 53.1 | 53.2 |
| Ti | T_N | 10.5 ± 1.1 | 11.7 | 10.1 | 8.2 |
| | R_N | 22.4 ± 2.2 | 67.8 | 17.8 | 18.6 |
| | T_E | 5.0 ± 0.5 | 3.2 | 4.0 | 3.9 |
| | R_E | 14.2 ± 1.4 | 47.6 | 9.7 | 11.8 |
| | ϕ_A | 80.8 ± 8.1 | 49.2 | 86.4 | 84.7 |

of 100 keV electrons through 25.4 μm -thick aluminium and titanium targets. Table I compares the experimental values with the results of calculations performed with TRIPOLI-4 v10 and with the development version of TRIPOLI-4. Geant4 calculation results from the literature [18] are also included for comparison.

The first observation is that the TRIPOLI-4 v10 results show little sensitivity to the target. This is probably connected to the underestimation of the mean free path for elastic scattering (Sec. II-B): indeed, an overestimated elastic cross section leads to excess multiple scattering. If electrons scatter too much and at too large angles, electron transport becomes akin to diffusion; under these conditions, one would expect the transmission and reflection coefficients to be essentially dominated by the geometry, which is the same in both cases (same thickness). Comparison with the experimental data makes it quite clear that this picture is largely erroneous.

The recent TRIPOLI-4 developments bring a substantial improvement. The salient features the experimental results are correctly reproduced, at least qualitatively. As a general trend, TRIPOLI-4 seems to slightly underestimate reflection and overestimate transmission. The Geant4 results are in better agreement with the experiment. These facts may probably be explained by considering that Geant4 singles out large-angle elastic scattering as a separate process¹. Backward elastic-scattering events, especially those that take place at small penetration depths, are expected to yield a sizeable contribution to reflection. It is clear that the effect of these collisions cannot be accurately modelled in the framework

¹Geant4's electron-transport algorithm falls in class II of Berger *et al.*'s ([19]) classification.

of an angular-straggling model, which by definition aims at capturing the mean effect of a large number of soft collisions.

IV. CONCLUSIONS

We have briefly presented a few recent TRIPOLI-4 developments concerning the treatment of the electromagnetic cascade, namely the implementation of a new model for the energy-differential bremsstrahlung cross section and a more careful treatment of the condensation of electron elastic cross sections into angular-straggling distributions. The impact of these developments is under study by comparing TRIPOLI-4 calculation results with experimental data and with the results of other transport codes. We have also presented the new charge-deposition score, which is useful for the simulation of self-powered neutron and gamma detectors, and the new thick-target-bremsstrahlung calculation mode.

ACKNOWLEDGMENT

TRIPOLI-4[®] is a registered trademark of CEA. Partial financial support from EDF (Électricité de France) is gratefully acknowledged.

REFERENCES

- [1] E. Brun, F. Damian, C. M. Diop, E. Dumonteil, F.-X. Hugot, C. Jouanne, Y. K. Lee, F. Malvagi, A. Mazzolo, O. Petit, J. Trama, T. Visonneau and A. Zoia, “TRIPOLI-4[®], CEA, EDF and AREVA reference monte carlo code”, *Ann. Nucl. Energy*, 2014, in press. DOI: 10.1016/j.anucene.2014.07.053.
- [2] M. J. Berger and S. M. Seltzer, “Bremsstrahlung and photoneutrons from thick tungsten and tantalum targets”, *Phys. Rev. C*, vol. 2, pp. 621–631, 2 Aug. 1970. DOI: 10.1103/PhysRevC.2.621.
- [3] Y. Peneliau, “Tests de validation de l’implémentation de la cascade électromagnétique dans le code de transport Monte Carlo TRIPOLI-4”, CEA-Saclay, France, Rapport DM2S SERMA/LEPP/RT/02-3186/A, Oct. 2002.
- [4] S. M. Seltzer and M. J. Berger, “Bremsstrahlung energy spectra from electrons with kinetic energy 1 keV–10 GeV incident on screened nuclei and orbital electrons of neutral atoms with $Z = 1-100$ ”, *Atom. Data Nucl. Data*, vol. 35, no. 3, pp. 345–418, 1986. DOI: 10.1016/0092-640X(86)90014-8.
- [5] J. Allison, K. Amako, J. Apostolakis, *et al.*, “Recent developments in Geant4”, *Nucl. Instrum. Meth. A*, vol. 835, pp. 186–225, 2016. DOI: 10.1016/j.nima.2016.06.125.
- [6] *Geant4 Physics Reference Manual*, version 10.2, Geant4 collaboration, Dec. 2015. [Online]. Available: <http://cern.ch/geant4/UserDocumentation/UsersGuides/PhysicsReferenceManual/fo/PhysicsReferenceManual.pdf>.
- [7] T. Goorley, M. James, T. Booth, *et al.*, “Initial MCNP6 release overview”, *Nucl. Technol.*, vol. 180, no. 3, pp. 298–315, Dec. 2012.
- [8] S. Goudsmit and J. L. Saunderson, “Multiple scattering of electrons”, *Phys. Rev.*, vol. 57, pp. 24–29, 1 Jan. 1940. DOI: 10.1103/PhysRev.57.24.
- [9] N. F. Mott, “The scattering of fast electrons by atomic nuclei”, *P. R. Soc. Ac*, vol. 124, no. 794, pp. 425–442, 1929. DOI: 10.1098/rspa.1929.0127.
- [10] G. Molière, “Theorie der Streuung schneller geladener Teilchen i: Einzelstreuung am abgeschirmten Coulomb-Feld”, *Z. Naturforsch.*, vol. 2, no. a, pp. 133–145, 1947.
- [11] —, “Theorie der Streuung schneller geladener Teilchen ii: Mehrfach- und Vielfachstreuung”, *Z. Naturforsch.*, vol. 3, no. a, pp. 78–97, 1948.
- [12] H. Feshbach, “The Coulomb scattering of relativistic electrons and positrons by nuclei”, *Phys. Rev.*, vol. 88, pp. 295–297, 2 Oct. 1952. DOI: 10.1103/PhysRev.88.295.
- [13] N. Sherman, “Coulomb scattering of relativistic electrons by point nuclei”, *Phys. Rev.*, vol. 103, pp. 1601–1607, 6 Sep. 1956. DOI: 10.1103/PhysRev.103.1601.
- [14] S. T. Perkins, D. E. Cullen and S. M. Seltzer, “Tables and graphs of electron-interaction cross sections from 10 eV to 100 GeV derived from the LLNL Evaluated Electron Data Library (EEDL), $Z = 1-100$ ”, Lawrence Livermore National Laboratory, Tech. Rep. UCRL-50400, Nov. 1991.
- [15] P. Ridoux, S. Kitsos, C. M. Diop, A. Assad and J. C. Nimal, “Improvement of gamma-ray S_n transport calculations including coherent and incoherent scatterings and secondary sources of bremsstrahlung and fluorescence: Determination of gamma-ray buildup factors”, *Nucl. Sci. Eng.*, vol. 123, no. 2, pp. 215–227, 1996.
- [16] D. Riz, “Calculation and use of multigroup cross sections including electron-photon cascade for a 3D Monte Carlo neutron-gamma transport code. Comparisons with MCNP-4B”, in *Proceedings to the 2000 ANS International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millennium (PHYSOR-2000)*, Pittsburgh, PA, USA, May 2000.
- [17] S. M. Seltzer and M. J. Berger, “Transmission and reflection of electrons by foils”, *Nucl. Instrum. Meth.*, vol. 119, pp. 157–176, 1974. DOI: 10.1016/0029-554X(74)90747-2.
- [18] O. Kadri, V. Ivanchenko, F. Gharbi and A. Trabelsi, “Incorporation of the Goudsmit–Saunderson electron transport theory in the Geant4 Monte Carlo code”, *Nucl. Instrum. Meth. B*, vol. 267, no. 23–24, pp. 3624–3632, 2009. DOI: 10.1016/j.nimb.2009.09.015.
- [19] M. J. Berger *et al.*, “Monte Carlo calculation of the penetration and diffusion of fast charged particles”, *Meth. Comp. Phys.*, vol. 1, pp. 135–215, 1963.