

Monte Carlo modelling of a track-etch detector using TOPAS

Pratyush Jha

1. Introduction:

Track-etch detectors are dosimeters that measure and record radiation exposure [1]. Being a dosimeter, it informs about the energies that the individual incident particles deposit on interacting with the detector. A track-etch detector, a.k.a. solid-state nuclear track detector (SSNTD), is a dielectric film of poly-allyl-diglycol-carbonate (PADC - $C_{12}H_{18}O_7$; a polymer), commonly known as CR-39, that form tracks when certain types of radiation pass through it. According to the radiochemical damage model [2], the interaction of a high-energy particle, which is capable of engaging with the CR-39 film, results in the creation of charged secondary particles (protons, oxygen, and carbon). When these secondaries travel through the detector volume, they break the long polymer chains into smaller fragments. These appear as nanoscopic tracks in the CR-39 film. The CR-39 film is sensitive to neutrons with energies above 100 keV and insensitive to thermal neutrons [3]. The tracks generated through the interaction of sensitive neutrons provide insights into the neutron dose accumulated within the detector. However, the nanoscopic tracks need further processing to be visualized. We use a process called chemical etching [4] to make these tracks visible under a microscope to be analyzed. The track density value, along with other track parameters, can then be assessed, which gives a measure of the dose that was deposited in the film.

Modelling and computational simulations of the radiation interactions with the track-etch detector can be an important step in understanding the response of the detector. Simulations can also be very helpful in planning real-world experiments efficiently. Simulation methods can be classified into three categories: (i) analytical method or mathematical modelling, (ii) modelling using artificial intelligence, and (iii) Monte Carlo (MC) modelling. Analytical modelling is fast and convenient to simulate ideal situations. However, as the complexity of the problem increases exponentially for real-world problems, analytical modelling is often not possible. Methods using Artificial Intelligence for modelling are in the development phase [5]. Monte Carlo Simulations, on the other hand, are considered the most accurate and flexible, and computationally efficient to model real-world scenarios in physics [5].

TOPAS (TOol for PArticle Simulation) MC is one of the software tools available for simulating particle passage through matter, particularly in radiation therapy [6]. It utilizes Geant4, a widely used toolkit for precise particle-matter interaction simulations [7]. TOPAS simplifies the process with a user-friendly interface and pre-configured setups for radiation therapy scenarios.

The objective of this project was to model and build a CR-39 detector in TOPAS and perform MC simulations to learn about the detector's response to neutrons of various

energies. We identified two tasks to be performed toward the completion of this objective. Therefore, in this report, I summarize the two Monte Carlo Simulation tasks that were performed using TOPAS.

1.1 Task-1: Simulation of the radiator-degrader setup to calculate the threshold energy values of the recoil protons: With the aim of getting accustomed to TOPAS, the first task was set to reproduce a specific result of Zaki-Dizaji et al. (2007). Our goal was to match the threshold energy values of the recoil protons generated in the radiator layer of a Radiator-Degrader-Detector (CR-39 detector) setup with the results [8] published in Table 1 of Zaki-Dizaji et al. (2007).

The research paper by Zaki-Dizaji et al. (2007) validates the use of a radiator-degrader-detector setup for increased efficiency to measure a broader range of neutron energies. In a radiator-degrader-detector setup, the incident neutrons on the radiator layer of polyethylene forms recoil nuclei that pass through a degrader layer of aluminum, which acts as a discriminator to allow protons of energy above a specific threshold to cross through and reach the detector layer. Threshold energy values for recoil protons generated in the radiator layer to cross through the degrader layer and get registered in the CR-39 detector were determined for different scattering angle values and nine different thicknesses of the degrader.

1.2 Task-2: Simulation of a track-etch detector (CR-39 film) for the calculation and comparison of the relative dose distribution of neutron secondaries in two experimental setups: We calculated the relative dose depositions of all the secondary particles, generated from neutrons, in a track-etch detector (CR-39 film). Two experimental setups were also compared by simulating a CR-39 film, with and without a water phantom, irradiated with an isotropic monoenergetic spherical source.

2. Methods:

2.1. Task-1: Simulation of the radiator-degrader setup to calculate the threshold energy values of the recoil protons:

The first task was to reproduce the results summarized in Table 1 of Zaki-Dizaji et al. (2007) and in this section, we describe their experimental setup that we adapted. Zaki-Dizaji et al.'s Table 1 summarize the threshold energy values of the recoil protons generated in the radiator layer (polyethylene) for different thicknesses of the degrader layer (aluminum). This setup is described in fig.1 (a) These thicknesses: 0, 20, 55, 90, 125, 210, 320, 440, and 520 μm make 9 different samples.

The threshold energy of recoil protons is the minimum energy of protons that get generated in the radiator layer, pass through the degrader layer, and get registered in the detector. The aluminum layer acts as a discriminator. As the thickness of the aluminum increases, protons need higher energy to pass through it, as can be observed from Table 1 of Zaki-Dizaji et al. (2007).

In our simulation a monoenergetic neutron source was defined at a distance of 4 cm from the degrader layer. Neutrons were made incident on the radiator-degrader arrangement at normal incidence. An optimal radiator thickness of 4 mm was considered, as with Zaki-Dizaji et al. (2007). In this case, the CR-39 detector layer was not simulated because the ZMinusSurface of the degrader (the surface which is supposed to be exposed to the detector) was declared as a Phase Space scorer. The scorer provided information about the particles' energy at the time of birth and the coordinates where it got created for all the secondary particles passing through this surface. Considering that the minimum energy required for a 100% detection efficiency for the protons is ~ 0.5 -8 MeV [9], the protons that got generated in the radiator layer and had energies greater than 0.5 MeV before leaving the aluminum layer were scored. The threshold energy of the proton was identified by observing the minimum energy value detected in the phase space scorer. This was repeated for 10 runs, each consisting of 30000 histories (the initial number of neutrons generated from the source). Fig. 1 summarizes the simulation setup.

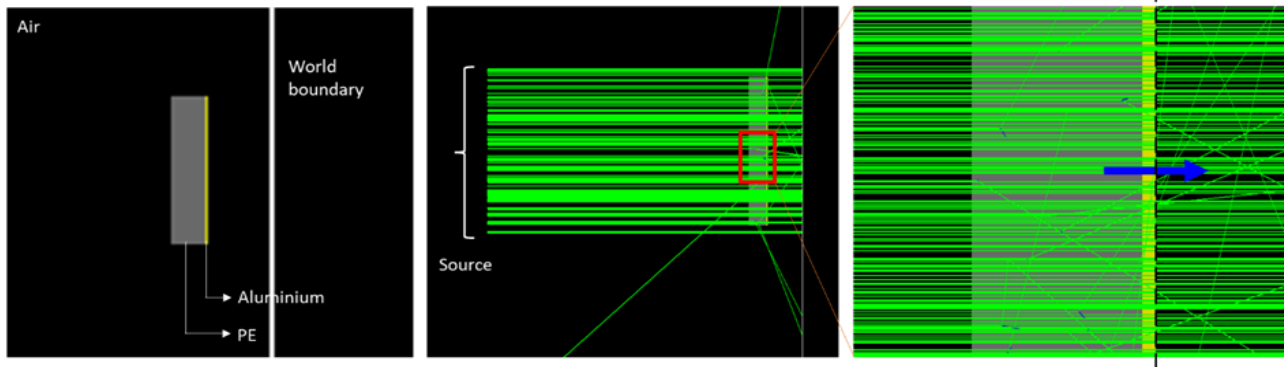


Fig. 1: (a) Detector construction: Radiator-Degrader-Detector setup, (b) Monoenergetic source of neutrons incident perpendicular to the polyethylene (PE) layer - 30,000 histories, (c) An enlarged image of a section of the detector during neutron irradiation, showing that the "ZMinusSurface" of the aluminum layer as the Phase Space Scorer.

2.2 Task-2: Simulation of a CR-39 film for the calculation and comparison of the relative dose distribution of neutron secondaries in two experimental setups

The second task described in this report aimed to obtain the relative dose distribution of the neutrons' secondary particles in a CR-39 film for two setups: one excluding the water phantom (setup-1, fig. 2) and the other consisting of a CR-39 film placed over a water box (setup-2, fig. 3) and compare the results.

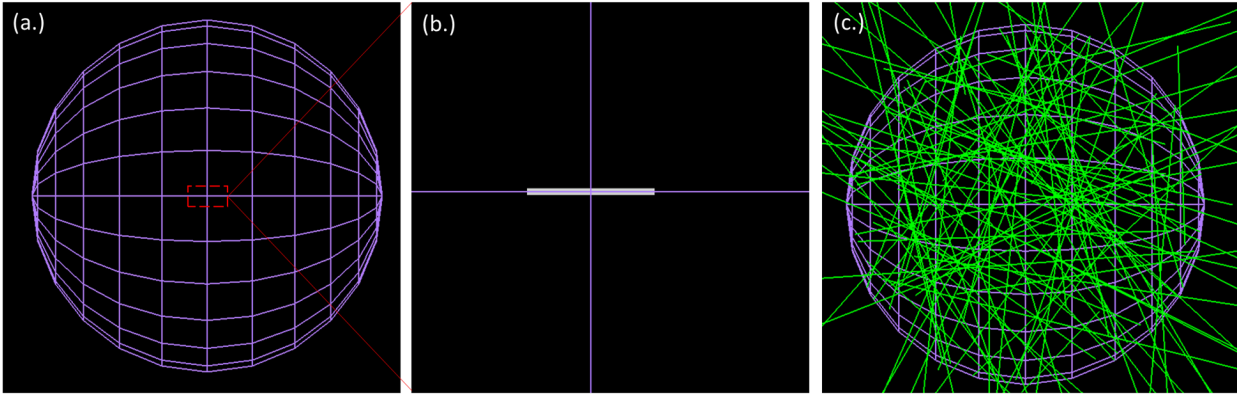


Fig. 2: Summarizing setup 1 of task 2: (a) The spherical surface depicted as a wireframe is the source, the red box shows the location of the CR-39 film placed at its center; (b) On magnifying the region in the red box, we find the CR-39 placed at the center of the spherical surface; (c) The spherical surface emits particles directed inside the sphere.

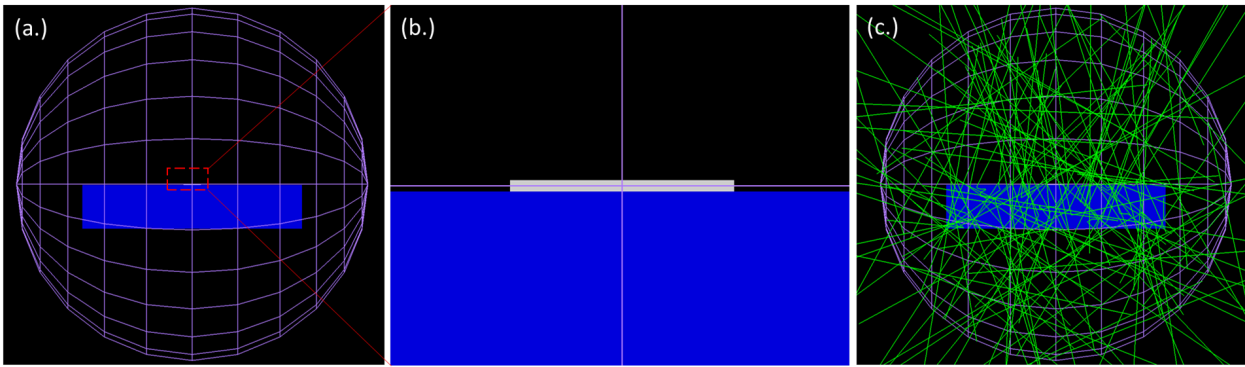


Fig. 3: Summarizing setup 2 of task 2: (a) The spherical surface depicted as a wireframe is the source, the red box shows the location of the CR-39 film placed on a water phantom (in blue) at its center; (b) On magnifying the region in the red box, we find the CR-39 placed on the water phantom; (c) The spherical surface emits particles directed inside the sphere.

The dimensions of the film and the water box were as follows:

- CR-39 film: 2.5 cm x 2 cm x 1 mm
- Water box: 25 cm x 25 cm x 10 cm

The radius of the spherical source was 20 cm.

The setup was irradiated with an isotropic spherical source of monoenergetic neutrons. The defined source is a surface source with the neutron beams directed “inside” the sphere to reduce the computation cost for simulating the less relevant neutrons going outside the sphere, which will not interact with the CR-39 film.

The CR-39 film was defined as the scoring volume using the scorer available in TOPAS-nBio - TsNtupleForCell. This scorer can provide an extensive summary of a particle's track and energy exchanges in the scoring volume.

Both the experimental setups were simulated to generate 10^6 neutrons, and the outputs were obtained in the ASCII format (.phsp and .header files) and analyzed using a Python script using the Pandas library [10].

3. Results:

3.1. Task-1: Simulation of the radiator-degrader setup to calculate the threshold energy values of the recoil protons:

Table 1 summarizes the results of our simulation. It consists of the threshold energy values of the recoil protons as given in Table 1 of Zaki-Dizaji et al. (2007), and as obtained from my work. We find that the threshold values from our simulation agree with those reported by Zaki-Dizaji et al. (2007).

Table 1: Threshold energy values as per Zaki-Dizaji et al. (2007) vs the threshold energy values obtained from our simulation

Aluminum thickness (μm)	Threshold energy (MeV) – Zaki-Dizaji et al. (2007)	Threshold energy (MeV) – This work
0	0.5	0.7
20	2.3	2.1
55	3.0	3.1
90	3.7	3.7
125	4.4	4.5
210	5.7	5.7
320	7.1	7.1
440	8.4	9.1
520	9.4	9.5

3.2 Task-2: Simulation of a CR-39 film for the calculation and comparison of the relative dose distribution of neutron secondaries in two experimental setups:

The result of task-2 of this project for setup-1 (CR-39 film without a water box) is summarized in Table 2.

Table 2: The relative dose deposition values of the particles in the CR-39 film for setup 1 (CR-39 film without a water box).

Secondary particles detected	Energy of the primary neutrons generated		
	5 MeV	10 MeV	15 MeV
Proton	0.83	0.78	0.73
Oxygen	0.04	0.05	0.06
Carbon	0.13	0.08	0.14
Carbon-13	0	0	0
Alpha Particle	0	0.03	0.03
Electron	0	0.05	0.03
PDG-1000040090	0	0	0
Others	0	0.01	0.01

The result of task-2 of this project for setup-2 (CR-39 film placed over a water box) is summarized in Table 3.

Table 3: The relative dose deposition values of the particles in the CR-39 film for Setup 2 (CR-39 film placed over a water box).

Secondary particles detected	Energy of the primary neutrons generated		
	5 MeV	10 MeV	15 MeV
Proton	0.84	0.79	0.63
Oxygen	0.06	0.06	0.08
Carbon	0.09	0.07	0.15
Carbon-13	0.01	0.01	0.01

Alpha Particle	0	0.05	0.1
Electron	0	0	0
PDG-1000040090	0	0.01	0.02
Others	0	0.01	0.01

4. Discussions:

For task-1, the results obtained by the Monte Carlo simulation using TOPAS for threshold values of the recoil protons generated in the radiator layer, cross through the aluminum degrader layer, and get registered in the CR-39 detector matched the results provided by Zaki-Dizaji et al. (2007) and hence I was successful in reproducing the already published results.

For task-2, simulations for the incident neutron energy values 5 MeV, 10 MeV, and 15 MeV for two different setups: Setup-1 and Setup-2, were successfully carried out to calculate the relative dose distribution of secondary particles from mono-energetic neutrons, formed in the simulations.

The next step in this project was to generate and compare the secondary particle spectra for the two setups for different energy values. However, it is currently incomplete because of the reasons discussed further:

Various methods to score the secondary particle spectra for the two setups were explored. However, it was finally concluded that no direct approach could be followed using the available TOPAS 3.9 and TOPAS-nBio 3.1 built-in scorers.

For the generation of secondary particle spectra, all the secondary particles falling on the track-etch detector need to be considered, whether or not they interact with the detector. Along with this, all the secondary particles formed from the primary neutrons inside the detector need to be considered. However, the tertiary particles formed from the secondary particles inside the detector film need to be rejected. The filters available in TOPAS 3.9 and TOPAS-nBio 3.1 were not able to give the desired result. Also, it was considered if the data obtained from the scorers could be used to figure out whether a particle is formed from a secondary particle or not using the particles' TrackID and the EventID. However, it was found that the particles' TrackID and EventID were not sufficient enough to find it out.

Hence, it is concluded that the only way to get the required spectra is to custom-build a scorer, by writing a Geant4 script as a TOPAS extension that can kill the “secondary particles as soon as they get registered” so as to avoid the formation of any further particles from these secondary particles.

5. Conclusion:

The importance of simulating a CR-39 detector using Monte Carlo modelling technique was identified, and two different setups with the CR-39 detector were simulated to obtain the relative dose deposition values secondary particles for three different energy values for the incident neutrons. It was identified that the currently available TOPAS' and TOPAS-nBio's in-built scorers are not sufficient to obtain secondary particle spectra for these setups, and there is a need to code a Geant4 extension to kill the secondary particles as soon as they get registered in the scorer.

References:

- [1] The use of solid-state nuclear track detectors in radiation dosimetry, medicine, and biology. (2002, October 9). The Use of Solid-state Nuclear Track Detectors in Radiation Dosimetry, Medicine and Biology - ScienceDirect. [https://doi.org/10.1016/0735-245X\(82\)90021-7](https://doi.org/10.1016/0735-245X(82)90021-7)
- [2] Becker K. DOSIMETRIC APPLICATIONS OF TRACK ETCHING. Topics in Radiation Dosimetry. 1972. pp. 79–142. doi:10.1016/b978-0-12-066501-3.50007-5
- [3] R. Pal, D. Sathian, J. V, A.K. Bakshi, M.P. Chougankar, Y.S. Mayya, V. Kumar, R. Babu, K. S., V.M. Joshi, Present status of fast neutron personnel dosimetry system based on CR-39 solid state nuclear track detectors, BARC External Technical Report, BARC/2011/E/015, BARC, India, 2011.
- [4] Bhagwat, A M. Solid state nuclear track detection : theory and applications. India: N. p., 1993. Web.
- [5] Ramos-Méndez. (2021, November). Lecture 1 Fundamentals of Monte Carlo [Video]. Retrieved May 14, 2023, from <https://ucsf.app.box.com/s/19lg45uncd3bx03jjodvgmxgeojnio9g/file/906177233076>
- [6] Faddegon B, Ramos-Mendez J, Schuemann J, McNamara A, Shin J, Perl J, Paganetti H, The TOPAS Tool for Particle Simulation, a Monte Carlo Simulation Tool for Physics, Biology and Clinical Research, Physica Medica, doi:10.1016/j.ejmp.2020.03.019
- [7] Agostinelli, S., Allison, J., Amako, K., Apostolakis, J., Araujo, H., Arce, P., Asai, M., Axen, D., Banerjee, S., Barrand, G., Behner, F., Bellagamba, L., Boudreau, J., Broglia, L., Brunengo, A., Burkhardt, H., Chauvie, S., Chuma, J., Chytracek, R., . . . Zschesche, D. (2003). Geant4—A simulation toolkit. *Nuclear Instruments and Methods in Physics*

Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 506(3), 250-303. [https://doi.org/10.1016/S0168-9002\(03\)01368-8](https://doi.org/10.1016/S0168-9002(03)01368-8)

[8] Zaki-Dizaji, H., Shahriari, M., & Etaati, G. (2007, September). Monte Carlo calculation of CR-39 efficiency for fast neutron detection using a combination of MCNP and SRIM codes, and comparison with experimental results. *Radiation Measurements*, 42(8), 1332–1334. <https://doi.org/10.1016/j.radmeas.2007.09.004>

[9] Rosenberg MJ, Séguin FH, Waugh CJ, Rinderknecht HG, Orozco D, Frenje JA, Johnson MG, Sio H, Zylstra AB, Sinenian N, Li CK, Petrasso RD, Glebov VY, Stoeckl C, Hohenberger M, Sangster TC, LePape S, Mackinnon AJ, Bionta RM, Landen OL, Zacharias RA, Kim Y, Herrmann HW, Kilkenny JD. Empirical assessment of the detection efficiency of CR-39 at high proton fluence and a compact, proton detector for high-fluence applications. *Rev Sci Instrum*. 2014 Apr;85(4):043302. doi: 10.1063/1.4870898. PMID: 24784597.

[10] McKinney, W., & others. (2010). Data structures for statistical computing in python. In *Proceedings of the 9th Python in Science Conference* (Vol. 445, pp. 51–56).