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Monte Carlo simulations of complex geometries and an optimal ^{60}cobalt source design using the integrated TIGER series (ITS 3.0)

Ali Bellou Mohamed [a], Joseph Silverman [a], Douglas E. Weiss [b], Mohamad Al-Sheikhly [a,*]

[a] *Laboratory for Radiation and Polymer Science, Nuclear Engineering Program, Material Science and Engineering Department, University of Maryland, College Park, MD 20742, United States*
[b] *3M Corporate Research Process Laboratory, 3M Center, St Paul, MN 55144-1000, United States*

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Abstract

In this work, the ITS 3.0/ACCEPT Monte Carlo code was used to determine the absorbed dose rates in a complex target consisting of various materials and densities. Dose rates in 512 sample vials packaged in dry ice and polyethylene were irradiated simultaneously using a ^{60}Co semi-cylindrical source array. The vials were distributed in two carriers set 1 m apart each holding 256 vials. For this specific target and source geometry, dose rate variations of $\pm 6\%$ were achieved among 226 vials in the first carrier, and among 203 vials exposed to a lower dose rate in the second carrier. Dose rate variations were found to depend only slightly on the backscatter contribution from the radiation vault walls.

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1. Introduction

The motivation for this work is to perform Monte Carlo simulations to aid in the design of a ^{60}Co source to meet specifications for delivering a specified uniform dose rate to a large number of glass vials ($\geqslant 200$) stacked in layers of a cylindrical sample carrier. The optimum configuration should meet the criterion that the contents of all sample vials have a dose rate difference of $\pm 5\%$ from the mean value for all vials within each sample carrier.

In gamma irradiation facilities the need often arises to irradiate a large number of samples simultaneously with a uniform radiation dose. In biomedical research, in particular, a large number of manufactured or cultured samples must be sterilized under controlled conditions [4] (such as low temperature where dry ice is needed) and strict dose variation limits. Tissue allografts frequently used in orthopedic reconstructive surgery have been found to lose their functionality when irradiated with doses above minimum sterilization requirements [5–7], and inadequate functionality [8] as well as infectious contamination [9] at low doses [8]. Dose rate variations are also potential problems; hence, there is the need to perform dose rate dependent studies on pathogen inactivation and tissue physical properties. This requires that many samples be irradiated simultaneously at different dose rates. Such experimental dose measurements for complex samples and carrier geometries in search of an optimum target, source and carrier configurations to achieve the desired dose rate within specified variation limits are costly and time consuming. In such cases, the use of the Monte Carlo method for precise dose calculations is essential.

In this work, the ITS 3.0/ACCEPT [2] was used to calculate the absorbed dose in complex geometries usually

* Corresponding author. Tel.: +1 301 405 5214; fax: +1 301 314 2029.
E-mail address: mohamad@eng.umd.edu (M. Al-Sheikhly).

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encountered in gamma irradiation research facilities. The ITS 3.0 Monte Carlo code system has been demonstrated [10–13,17,18] to be a very accurate dose prediction tool, one that is benchmarked against experimental results. Dose mapping results in gamma irradiators of various source designs and target geometries using another Monte Carlo code, MCNP [16], have been reported [14,15] and found to agree well with experimental results. In this work, we make minor approximations in applying the code but nevertheless calculate in great detail the absorbed dose rate in complex geometries relative to this problem. This work also shows that once certain complex target geometry and source configurations are found to meet dose rate variation limits in a carrier fully loaded with vials, dose rate variation limits can be calculated in partially loaded carriers. Dose rate experimental measurements only in extreme locations of individual vials in a smaller loading, is a sufficient basis for calculation of precise dose rates in all locations without the need to perform detailed time-consuming simulations and/or measurements for each vial.

2. Monte Carlo simulations

Monte Carlo simulations were performed using ITS 3.0/ACCEPT transport code. ITS 3.0[1] is a system of general purpose time-independent, multimaterial, multidimensional coupled electron/photon Monte Carlo transport codes that combine collisional transport with transport in an externally applied macroscopic electric and magnetic fields over the energy range from 1 GeV to 1 keV. The code is capable of simulating the production and transport of electrons, positrons and gammas. The electron/positron interactions include: energy loss straggling, elastic scattering, production of knock-on electrons, impact ionization followed by production of fluorescence X-rays or Auger electrons, Bremsstrahlung production and the production of annihilation radiation. The photon interactions include: photoelectric absorption with the production of photoelectrons, Auger electrons and fluorescence X-rays, incoherent scattering, with the production of scattered electrons, coherent scattering and pair production.

The ITS 3.0 code system consists of eight codes; standard, P and M codes. TIGER, CYLTRAN and ACCEPT are the standard codes in one, two/three and three dimensions, respectively. The P codes (TIGERP, CYLTRANP and ACCEPTP) are the versions of the code that include a more detailed ionization/relaxation model. The M codes (CYLTRANM and ACCEPTM) are the versions that combine collisional transport with transport in electric and magnetic fields [1]. Further description of the ITS code system can be found in the literature [2,1,3].

[1] Can be obtained from the Radiation Shielding Information Computational Center (RSICC), Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA.

2.1. The ITS 3.0 Monte Carlo code system

The ITS 3.0 consists of four essential elements: (1) the electron/photon cross-section data file (XDATA), (2) the cross-section generation program (XGEN) file, (3) the Monte Carlo program file (ITS) and (4) the machine portable update emulator (UPEML). The executable programs are: XGEN; ACCEPT, CYLTRAN and TIGER; and UPEML. For problems that involve large scale and very complex geometries, some parameters in the Monte Carlo program file have to be increased with the use of the machine portable update emulator (UPEML) to generate a new source file that can later be compiled using a FORTRAN 77 compiler. The UPEML program is a utility for maintaining and manipulating the ITS 3.0 source code in a controlled error free manner to modify the original ITS code system or just increase or decrease some of the code parameters. If a parameter needs to be increased, the Monte Carlo program will generate an error message instructing the user to increase a parameter or parameters in order for the Monte Carlo program to run successfully. For example, in our problem, the number of input zones exceed the default value for the ITS 3.0/ACCEPT so we increased the INIZON parameter to a higher value.

2.2. Model geometry

The geometry model includes the source and target(s) that comprise more than 2300 solid objects. This is a considerable task and a systematic strategy to construct the geometry model was adopted to minimize subtle geometry errors. At this time, the ITS 3.0/ACCEPT has no CAD support and the model geometry had to be built manually. We were successful in building the entire problem geometry by means of a systematic numbering system that made it easier to debug geometry errors. In addition, we used SABRINA [19], to display the final ACCEPT model geometry and thereby reveal geometry errors. Because the input file for our model is an 80-page text file, we show here only a three-vial input to serve as a scaled-down version of the geometry and its attendant problems. The union operator, "OR", was extensively used to combine all "air" and "glass" input zones in the problem geometry, thereby leading to a substantial reduction in the sizes of ACCEPT's input and output files. Only the "water" zones were defined explicitly as those in which the dose rate is tallied. Appendix A.1 lists the ACCEPT input file for the three-vial model. Appendix A.2 shows the zone description strategy. A line drawing of the three-vial problem geometry rendered by SABRINA is shown in Fig. 1.

2.3. Source description

The source was modeled as ten line sources (pencils) of total initial activity of 108 kCi of ^{60}Co of average energy of 1.25 MeV. The use of an average energy of 1.25 MeV is to reduce the computational overhead. The difference in the