Designation: E2232 – 16

Standard Guide for Selection and Use of Mathematical Methods for Calculating Absorbed Dose in Radiation Processing Applications[1]

This standard is issued under the fixed designation E2232; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This guide describes different mathematical methods that may be used to calculate absorbed dose and criteria for their selection. Absorbed-dose calculations can determine the effectiveness of the radiation process, estimate the absorbed-dose distribution in product, or supplement or complement, or both, the measurement of absorbed dose.

1.2 Radiation processing is an evolving field and annotated examples are provided in Annex A6 to illustrate the applications where mathematical methods have been successfully applied. While not limited by the applications cited in these examples, applications specific to neutron transport, radiation therapy and shielding design are not addressed in this document.

1.3 This guide covers the calculation of radiation transport of electrons and photons with energies up to 25 MeV.

1.4 The mathematical methods described include Monte Carlo, point kernel, discrete ordinate, semi-empirical and empirical methods.

1.5 This guide is limited to the use of general purpose software packages for the calculation of the transport of charged or uncharged particles and photons, or both, from various types of sources of ionizing radiation. This standard is limited to the use of these software packages or other mathematical methods for the determination of spatial dose distributions for photons emitted following the decay of ^{137}Cs or ^{60}Co, for energetic electrons from particle accelerators, or for X-rays generated by electron accelerators.

1.6 This guide assists the user in determining if mathematical methods are a useful tool. This guide may assist the user in selecting an appropriate method for calculating absorbed dose. The user must determine whether any of these mathematical methods are appropriate for the solution to their specific application and what, if any, software to apply.

NOTE 1—The user is urged to apply these predictive techniques while being aware of the need for experience and also the inherent limitations of both the method and the available software. Information pertaining to availability and updates to codes for modeling radiation transport, courses, workshops and meetings can be found in Annex A1. For a basic understanding of radiation physics and a brief overview of method selection, refer to Annex A3.

1.7 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory requirements prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E170 Terminology Relating to Radiation Measurements and Dosimetry

E482 Guide for Application of Neutron Transport Methods for Reactor Vessel Surveillance

2.2 *ISO/ASTM Standards:*[2]

51707 Guide for Estimating Uncertainties in Dosimetry for Radiation Processing

2.3 *International Commission on Radiation Units and Measurements Reports:*[3]

ICRU Report 85a Fundamental Quantities and Units for Ionizing Radiation

2.4 *United States National Institute of Standards and Technology:*[4]

NIST Technical Note 1297 (1994 edition) Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results

3. Terminology

3.1 *Definitions:*

[1] This guide is under the jurisdiction of ASTM Committee E61 on Radiation Processing and is the direct responsibility of Subcommittee E61.04 on Specialty Application.

Current edition approved Dec. 1, 2016. Published January 2017. Originally approved in 2002. Last previous edition approved in 2010 as E2232-10. DOI: 10.1520/E2232-16.

[2] For referenced ASTM and ISO/ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] Available from International Commission on Radiation Units and Measurements, 7910 Woodmont Ave., Suite 800, Bethesda, MD 20815 USA.

[4] Available as a download from the NIST web site at: http://physics.nist.gov/Pubs/guidelines/TN1297/tn1297s.pdf.

3.1.1 *accuracy (VIM)*—closeness of agreement between a measured quantity value and a true quantity value of a measurand.

3.1.2 *benchmarking*—comparing model predictions to independent measurements or calculations under similar conditions using defined criteria of uncertainty.

3.1.2.1 *Discussion*—Benchmarking is a prerequisite before routine use of a mathematical model. Refer to 8.1 and Annex A5.

3.1.3 *biasing (in a Monte Carlo simulation)*—adjustment of the source particle selection or the transported particle weight, or both, in a statistically valid manner so as to increase the particles in a region where the detector response is most important.

3.1.3.1 *Discussion*—Biasing is a method used to reduce the estimated uncertainty or computer run times of Monte Carlo simulations. Monte Carlo simulations using the natural probabilities of physical events may require unacceptably long run times to accumulate statistics for rare events. The simulated probabilities may be altered to achieve the uncertainty goals for the simulation in acceptable run times by biasing the sampling from the probability distributions. The number of particles tracked and the particle weights may be adjusted so as to ensure a statistically valid sample from the probability distributions. Appropriate biasing requires a detailed knowledge of the model and the influence of rare events. As with all simulations, results should be compared with benchmark measurements or simulation results originated by a different code.

3.1.4 *build-up factor*—ratio of the total value of a specified radiation quantity (such as absorbed dose) at any point in that medium to the contribution to that quantity from the incident un-collided radiation reaching that point.

3.1.4.1 *Discussion*—The concept of build-up applies to the transport of photons.

3.1.5 *deterministic method*—a mathematical method using transport equations to directly calculate the radiation field over all space as a function of radiation source and boundary conditions.

3.1.5.1 *Discussion*—The point kernel and discrete ordinate methods are examples of deterministic methods.

3.1.6 *discrete ordinate method*—a deterministic method for approximate numerical solution of the transport equation in which the direction of motion is divided into a finite number of discrete ordinate angles.

3.1.6.1 *Discussion*—In the discrete ordinates approximation, the transport equation becomes a set of coupled equations, one for each discrete ordinate. Particle behaviors along paths intermediate to described paths are approximated by a weighted average (numerical quadrature) of adjacent paths (**1**).[5] The method is useful for both electron and photon sources when appropriate assumptions can be made.

3.1.7 *empirical method*—a method derived from fitting an approximating function to experimental data or Monte Carlo calculation result.

3.1.7.1 *Discussion*—Empirical models are generally developed by fitting equations (for example, polynomial) to experimental data or simulation output derived from another mathematical method.

3.1.8 *history (of a particle)*—record of all simulated interactions along particle's track as used in stochastic simulations (for example, Monte Carlo).

3.1.8.1 *Discussion*—A particle history begins with the starting position, energy and direction of a particle, follows all its interactions, and terminates in one of several outcomes such as absorption, escape from the boundary of the problem, or reaching a cut-off limit (such as a cut-off energy). A particle history is the systematic generation of a random, simulated particle track that is obtained according to the known physical interactions of either electrons or photons with the material being traversed. History and particle history are considered synonymous.

3.1.9 *mathematical method*—a method of solution of an electron or photon transport problem, or both, using algebraic relations and mathematical operations to represent the system and its dynamics.

3.1.10 *mathematical model*—a mathematical description of a physical problem based on physical laws or empirical correlation, or both.

3.1.11 *Monte Carlo method*—a simulation method used for calculating absorbed dose, energy spectra, charge, fluence and fluence rate in a volume of interest using a statistical summary of the radiation interactions.

3.1.11.1 *Discussion*—A Monte Carlo calculation consists of running a large number of particle histories (simulations) until some acceptable statistical uncertainty in the desired calculated quantity (such as dose) has been reached. This calculation method is suitable for problems involving either electrons or photons or both. This technique produces a probabilistic approximation to the solution of a problem by using statistical sampling techniques. See also *stochastic* and *history*.

3.1.12 *numerical convergence*—process in which the iterative solution of an equation or set of equations changes by less than some defined value.

3.1.12.1 *Discussion*—The mathematical equations describing a problem are often so complex that an analytical (algebraic) solution is not possible. The solution of the equations can be estimated by an iterative process of progressively refining approximate solutions at a grid of discrete locations. A consistent set of solutions arrived at by this method achieves numerical convergence. Convergence may not be obtained if the discrete locations are too widely separated (that is, the grid is too coarse).

3.1.13 *point kernel method*—a deterministic method for calculating dose based on integrating the contributions from point sources.

3.1.13.1 *Discussion*—The point kernel method is typically used for photon transport applications. The radiation source is modeled as a large set of point sources. The absorbed dose,

[5] The boldface numbers in parentheses refer to the list of references at the end of this standard.

dose equivalent or exposure is estimated at a dose point by integrating the contribution from each of the point sources. A multiplicative value (the semi-empirical build-up factor) is used to account for the contribution from scattered (indirect) radiation from regions not in the direct path between the source point and field point.

3.1.14 *radiation field*—a function describing the particle density and the distributions of energy, direction and particle type at any point.

3.1.15 *radiation transport theory*—an analytical description of the propagation of a radiation field according to the physical laws governing the interaction of radiation with matter.

3.1.15.1 *Discussion*—In its most general form, transport theory is a special branch of statistical mechanics, which deals with the interaction of the radiation field with matter.

3.1.16 *semi-empirical model*—an empirical model in which the fitting parameters are constrained so that the model satisfies one or more physical laws or rules.

3.1.16.1 *Discussion*—The satisfaction of such physical rules may enable the model to be applicable over a wide range of energies and materials.

3.1.17 *spatial mesh*—subdivision of the radiation interaction volume of interest into a grid of discrete spatial elements for performing a transport calculation.

3.1.18 *statistical component of uncertainty*—component of uncertainty evaluated by statistical analysis of a series of calculated values.

3.1.18.1 *Discussion*—The inherent sampling uncertainty of the Monte Carlo method can be estimated as a statistical uncertainty by applying statistical sampling techniques to the number of simulated histories. For calculations without biasing, the statistical uncertainty scales as the reciprocal of the square root of the number of histories.

3.1.19 *stochastic methods*—methods using mathematical equations containing random variables to describe or summarize the physical processes in the system being studied. A random variable is a variable whose value is a function of a statistical distribution of random values.

3.1.19.1 *Discussion*—The Monte Carlo method is the only stochastic method discussed in this guide. See also *Monte Carlo* and *history*.

3.1.20 *non-statistical component of uncertainty*—component of uncertainty evaluated by means other than statistical analysis of a series of calculated values.

3.1.20.1 *Discussion*—There are non-statistical components of uncertainties associated with the necessary simplifying assumptions needed to approximate the physical paths of electrons in the model and uncertainties in the cross-sections for the different interactions. These uncertainties can be estimated by analytical techniques. A non-statistical component of uncertainty could result from the difference in geometry and material composition of the modelled irradiator versus the actual irradiator. Other sources of non-statistical component of uncertainty are the inadequate description of the problem and approximations to actual physics.

3.1.21 *transport equation*—an integro-differential equation describing the motion of particles or radiation through a medium.

3.1.21.1 *Discussion*—The transport equation contains various terms corresponding to sources of particles, particle streaming and particle scattering in and out of an infinitesimal volume of phase space.

3.1.22 *uncertainty of calculation result*—non-negative parameter associated with the result of a calculation that characterizes the spread of values that could reasonably be attributed to the derived quantity.

3.1.22.1 *Discussion*—Like absorbed-dose measurement, the absorbed-dose calculation should also be accompanied by an estimate of uncertainty.

3.1.23 *validation*—accumulation of documented experimental evidence, used to demonstrate that the mathematical method is a reliable prediction technique.

3.1.23.1 *Discussion*—Validation compares a code or theory with results of an appropriate experiment.

3.1.24 *verification*—confirmation by examination of evidence that the mathematical method has been properly and successfully applied to the problem.

3.1.24.1 *Discussion*—It is important to know the type of radiation sources, geometries, energies, etc. for which a code has been validated. The calculated results will also depend on quantities at the user's disposal such as cut-off energy (for Monte Carlo) or mesh size (for discrete ordinate methods). Verification demonstrates that theory was implemented in the way intended, and that the simulation was performed in accordance with its requirements and specifications.

3.1.25 *zoning*—The geometric description used to break up a larger region into smaller segments in which to calculate the dose.

3.1.25.1 *Discussion*—Partitioning a zone into smaller segments is referred to as subzoning.

3.2 Definitions of other terms used in this standard that pertain to radiation measurement and dosimetry may be found in Terminology E170. Definitions in Terminology E170 are compatible with ICRU 85a; those documents, therefore, may be used as alternative references.

4. Significance and Use

4.1 *Use as an Analytical Tool*—Mathematical methods provide an analytical tool to be employed for many applications related to absorbed dose determinations in radiation processing. Mathematical calculations may not be used as a substitute for routine dosimetry in some applications (for example, medical device sterilization, food irradiation).

4.2 *Dose Calculation*—Absorbed-dose calculations may be performed for a variety of photon/electron environments and irradiator geometries.

4.3 *Evaluate Process Effectiveness*—Mathematical models may be used to evaluate the impact of changes in product composition, loading configuration, and irradiator design on dose distribution.

4.4 *Complement or Supplement to Dosimetry*—Dose calculations may be used to establish a detailed understanding of dose distribution, providing a spatial resolution not obtainable through measurement. Calculations may be used to reduce the number of dosimeters required to characterize a procedure or process (for example, dose mapping).

4.5 *Alternative to Dosimetry*—Dose calculations may be used when dosimetry is impractical (for example, granular materials, materials with complex geometries, material contained in a package where dosimetry is not practical or possible).

4.6 *Facility Design*—Dose calculations are often used in the design of a new irradiator and can be used to help optimize dose distribution in an existing facility or radiation process. The use of modeling in irradiator design can be found in Refs (**2-7**).

4.7 *Validation*—The validation of the model should be done through comparison with reliable and traceable dosimetric measurements. The purpose of validation is to demonstrate that the mathematical method makes reliable predictions of dose and other transport quantities. Validation compares predictions or theory to the results of an appropriate experiment. The degree of validation is commensurate with the application. Guidance is given in the documents referenced in Annex A2.

4.8 *Verification*—Verification is the confirmation of the mathematical correctness of a computer implementation of a mathematical method. This can be done, for example, by comparing numerical results with known analytic solutions or with other computer codes that have been previously verified. Verification should be done to ensure that the simulation is appropriate for the intended application. Refer to 3.1.24.

NOTE 2—Certain applications of the mathematical model deal with Operational Qualification (OQ), Performance Qualification (PQ) and process control in radiation processing such as the sterilization of healthcare products. The application and use of the mathematical model in these applications may have to meet regulatory requirements. Refer to Section 6 for prerequisites for application of a mathematical method and Section 8 for requirements before routine use of the mathematical method.

4.9 *Uncertainty*—An absorbed dose prediction should be accompanied by an estimate of overall uncertainty, as it is with absorbed-dose measurement (refer to ISO/ASTM 51707 and NIST Technical Note 1297). In many cases, absorbed-dose measurement helps to establish the uncertainty in the dose calculation.

4.10 This guide should not be used as the only reference in the selection and use of mathematical models. The user is encouraged to contact individuals who are experienced in mathematical modelling and to read the relevant publications in order to select the best tool for their application. Radiation processing is an evolving field and the references cited in the annotated examples of Annex A6 are representative of the various published applications. Where a method is validated with dosimetry, it becomes a benchmark for that particular application.

5. Classification of Mathematical Methods and General Application

5.1 Mathematical methods for radiation transport can be used to estimate the absorbed dose to a small volume or point. The dose distribution within the entire product can be determined by calculations at different points within the product.

5.2 *Types of Methods*—Four general types of methods are in use: Monte Carlo, deterministic, semi-empirical and empirical. Both Monte Carlo and deterministic methods are based on the detailed physics of the interaction of radiation with matter.

5.2.1 Monte Carlo methods involve simulating paths of a finite number of photons or electrons and estimating dose by summing and averaging the histories of many energy deposition events.

5.2.2 Deterministic methods use equations describing the transport of radiation in matter to perform a direct estimate of the total radiation field, absorbed dose and other responses.

5.2.3 Empirical and semi-empirical methods are based on statistical relationships of measurements or calculations for a particular system.

5.3 *Monte Carlo Method*—The Monte Carlo method simulates the paths of particles such as electrons and photons from the source to the dose volume. See Note 1, Refs (**8-19**) and Annex A1 for examples and codes. See also A3.3 and A3.4.4 for brief discussions of the physics of electron and photon transport and the Monte Carlo method respectively.

5.3.1 *Advantages*—Unlike other methods, the Monte Carlo method can, in principle, account for all interactions and provide a realistic simulation of actual all scattering and energy loss events. All contributions to the absorbed dose can be taken into account including electron and photon scattering from nearby objects. (See Note 3.) In addition, the Monte Carlo method has the great advantage of being the method most capable of simulating the actual radiation transport in complex three-dimensional geometry.

NOTE 3—Such objects could be structures outside the system of irradiated material(s) for which the dose distribution is to be calculated. For example, these might include shielding layers, photon beam collimators, e-beam accelerator heads, or walls of concrete or lead surrounding a ^{60}Co radiation source.

5.3.2 *Disadvantages*—Because electrons (including those generated by photons) in the energy range of 50 keV to 10 MeV undergo large numbers of scattering events, exact simulation of all photon and electron paths is not feasible or practical. Instead, approximate electron paths are employed, as in the so-called “condensed history Monte Carlo method” (**20 and 21**). For electrons, approximate artificial trajectories using large path length steps and a multiple-scattering approach to particle deflections are employed in standard Monte Carlo codes. (See Annex A1.) The standard Monte Carlo codes listed in Annex A1 and Refs (**8-19**) use this condensed history approach. However, such approximate paths may lead to significant errors, particularly at locations where transport across surfaces or material interfaces is important. See Note 4.

NOTE 4—In some Monte Carlo codes (17), improved accuracy near material boundaries has been obtained using shorter paths near interfaces between different materials.

NOTE 5—To reduce computational time, limits to the problem may be specified, such as physical boundaries and energy cut-offs, when the contributions to the problem made outside of these boundaries are no longer expected to be significant. Variance reduction techniques help to improve the rate of numerical convergence but require a sophisticated understanding of probability distributions.

5.3.2.1 One of the main difficulties with this method is its application to geometries that create reductions in fluence spanning orders of magnitude (for example, thick shields, complicated mazes, and air cavities).

5.3.2.2 Another difficulty is that, when the dose volume is small, Monte Carlo calculations may require variance reduction techniques. This type of problem may occur when attempting to calculate the dose within a dosimeter volume (for example, an 18-μm thick thin film or a layered 100-μm thick radiochromic film).

5.3.2.3 Calculations of dose should provide a range of dose values over a region near where the dose is to be measured. This is to permit estimation of the effect of variations in the location/orientation of a dosimeter in that region. This determines the dose sensitivity associated with placement of the dosimeter and allows determination of this type of error.

5.3.3 *Statistical Uncertainty*—The inherent uncertainty in the calculated value of dose due to sampling in the Monte Carlo method can be estimated by applying statistical sampling techniques to the number of histories. For calculations without biasing, the statistical uncertainty scales as the reciprocal of the square root of the number of histories run.

5.3.3.1 Special care must be taken when using variance reduction techniques which are used to increase statistics in an otherwise poorly populated phase space (for example, shielding calculation where only high energy photons are tracked through the shield). This is accomplished by introducing sampling probabilities which may be highly varying and have an adverse effect on the convergence of Monte Carlo calculations.

5.3.4 *Non-statistical Component of Uncertainty*—These uncertainties can be estimated by analytical techniques, which may include sensitivity analysis (changing a value of a parameter by an amount related to its uncertainty and rerunning the calculation to compare the results. Various elements of the calculation can be validated with dosimetry.

NOTE 6—There is great potential for large discrepancies in results because there is no estimate of non-statistical component of uncertainty resulting from software. Refer to Section 9. Construction of an uncertainty budget is recommended.

5.4 *Deterministic Methods*—These methods use analytical equations to summarize radiation fluence rate through target materials. Such complex equations cannot be solved directly but must be solved iteratively in the computer calculations.

5.4.1 *Discrete Ordinates Methods*—These methods have been used for both electron and photon sources (**22 and 23**). This name is given to several closely related techniques for obtaining approximate solutions to the transport equations that contain both integral and partial derivative terms. Various methods have been developed to solve these equations (**24**). All of these methods place limits on the angular variable such that the incident radiation is represented as streaming only along a finite number of directions rather than all possible directions as contained in the transport equation. Extension of this technique to 2-D and 3-D has been done by several authors (**25**).

5.4.2 *Point Kernel Methods*—Point kernel methods are used mainly for photon transport problems (**26**). In point kernel methods, the radiation source volume is approximated by a number of isotropic source points. The absorbed dose at each dose point is obtained by summing the dose contribution from all source points. The calculation takes into account the distance between the dose point and the source point and approximates the scatter within the intervening product through the use of a build-up factor. Build-up factors are theoretically calculated and sometimes fitted to empirical functions. These factors provide an approximation for the contribution of scattered photons from surrounding material. Approximations are also required to account for the energy spectrum and variations in the atomic number in different intervening or scattering materials.

NOTE 7—There are a number of general databases available for the photon buildup factors needed for these codes (Annex A1).

5.4.3 *Advantages*—Deterministic methods may be faster than Monte Carlo, and can be benchmarked against dosimetry.

5.4.4 *Disadvantages*—Deterministic methods give no innate estimate of statistical uncertainty. Iterative solution methods may be susceptible to numerical convergence errors and oscillatory solutions.

5.4.5 *Uncertainties*—There are three sources of uncertainties in deterministic models. These are *(1)* the approximations used to create physical models and cross-sections (for example, energy straggling is neglected in deterministic methods), *(2)* the effect of representing a continuous problem in space, angle and energy with a finite mesh in all these variables and *(3)* truncation error due to a finite number of discrete ordinates.

5.4.6 The accuracy of the point kernel treatment may be comparable to that of a Monte Carlo calculation for configurations where the point kernel approximation is valid (**27**).

5.5 *Empirical and Semi-empirical Methods:*

5.5.1 *Empirical*—Empirical methods typically involve fitting analytical functions to experimental measurements (or to calculations using other methods). The model equations are typically specific to a particular radiation facility and their predictive capabilities are not generally transferable to other facilities or products. Some simple equations exist for calculating the range of electrons in condensed matter (**28**), electron energy loss (**29**) and depth-dose relationships in various materials (**30**).

5.5.2 *Semi-Empirical*—These are empirical methods in which the fitting parameters are constrained so that the model satisfies one or more physical laws or rules. These methods provide a more generally applicable mathematical model than the empirical method and are adjustable to physical parameters of the facility, source and products, such as energy, density and composition. In general, these are software-based programs with variable parameter inputs. Equations, codes and databases are available (**31-34**).

5.5.3 *Advantages*—Empirical and semi-empirical models are fast and do not require cross-sections, build-up factors and zoning since they are implicitly included in the coefficients of the model. No special knowledge, such as needed for Monte Carlo or deterministic methods, is required. Semi-empirical models may be applicable to multiple facilities.

5.5.4 *Disadvantages*—Empirical methods are likely to be very limited in their application. Generally, empirically derived equations cannot be transferred to other sites or irradiation applications, or both, that were not part of the original database used to generate the model. These methods may be difficult to implement for systems with complicated geometry.

NOTE 8—Although empirical or semi-empirical codes may give some useful guidance, modern Monte Carlo codes on modern platforms are often very fast in these types of applications.

5.5.5 *Uncertainties*—Uncertainty in both methods is influenced by factors such as lack of homogeneity in the product, dosimeter location and uncertainty associated with dose measurements.

6. Prerequisites for Application of a Mathematical Method

6.1 *Facility and Related Geometry Considerations:*

6.1.1 Detailed drawings of irradiation facility equipment, source-related equipment and associated geometries, should be obtained, physically verified, and documented. Examples of gamma irradiation facilities are given in Figs. 1 and 2.

NOTE 9—Fig. 1 shows a physical model of a typical gamma irradiator with product in aluminum totes. For clarity, four totes and part of the source shroud have been removed. The tote irradiator uses a shuffle-and-dwell concept. Each product tote is irradiated for a defined period of time before it is moved to the next irradiation position. The source rack containing the radiation sources is shown (**36**).

NOTE 10—Fig. 2 shows a photograph on the left of a research carrier and the graphical user interface window of a mathematical model shown on the right photograph. All product is contained in aluminum totes. For the research carrier, product is brought into the radiation chamber and irradiated for a defined period of time, and then leaves the irradiation chamber. The graphical user interface shows ray tracing between the radiation source (1) and the dose volume (2) (**36**).

6.1.2 Detailed drawings of materials to be irradiated (products, targets) and their associated geometries, with physical verification of the same (composition of constituents, densities) should be collected and documented.

6.1.3 The type of source(s) present (electrons, photons), source energy spectrum, source output angular distribution, source size (point or distributed, diffuse source with variable activity etc.) and the number of sources should be specified and documented.

NOTE 11—In the case of gamma-ray sources (for example, ^{60}Co sources), the photon energy spectrum may be difficult to obtain experimentally or estimate theoretically. In general, for photons with energies 200 keV and above, a broad low energy contribution to the spectrum is created via Compton scattering.

6.2 *Personnel*—Trained personnel should be involved in all aspects of model development, program execution, data reduction and the evaluation of results. There is no standard set of qualifications that can be recommended. Interaction of personnel with all phases of the modeling exercise should be documented according to the end-user's policy and procedural

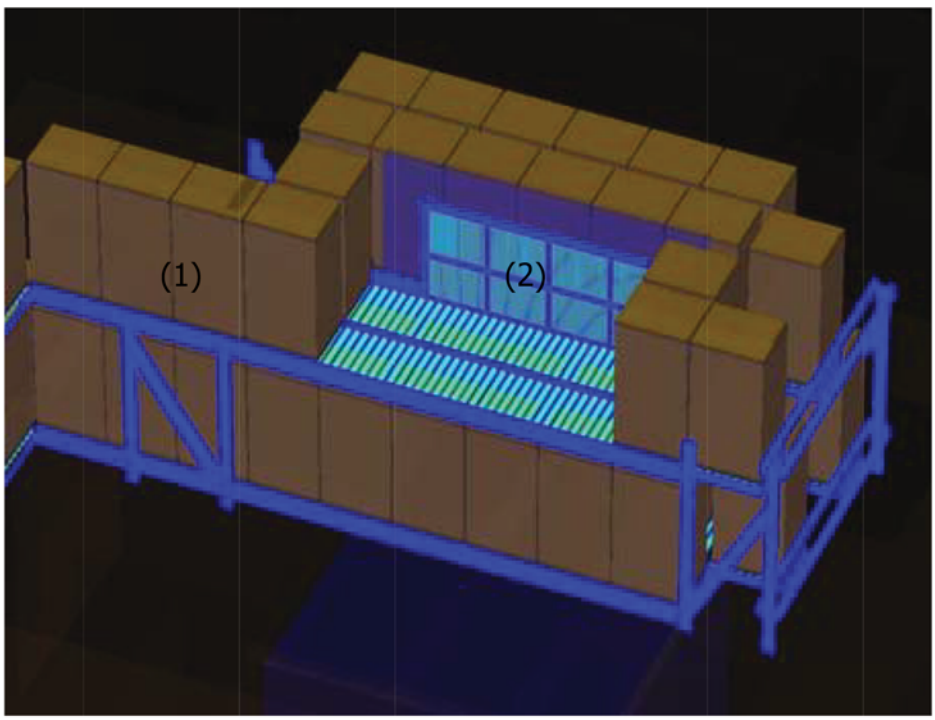

FIG. 1 Solid Model of a modified Nordion JS9600 Irradiator with a two layer roller conveyor, showing the product totes (1) and the radiation source (2). The model was developed using EGSPP (35)

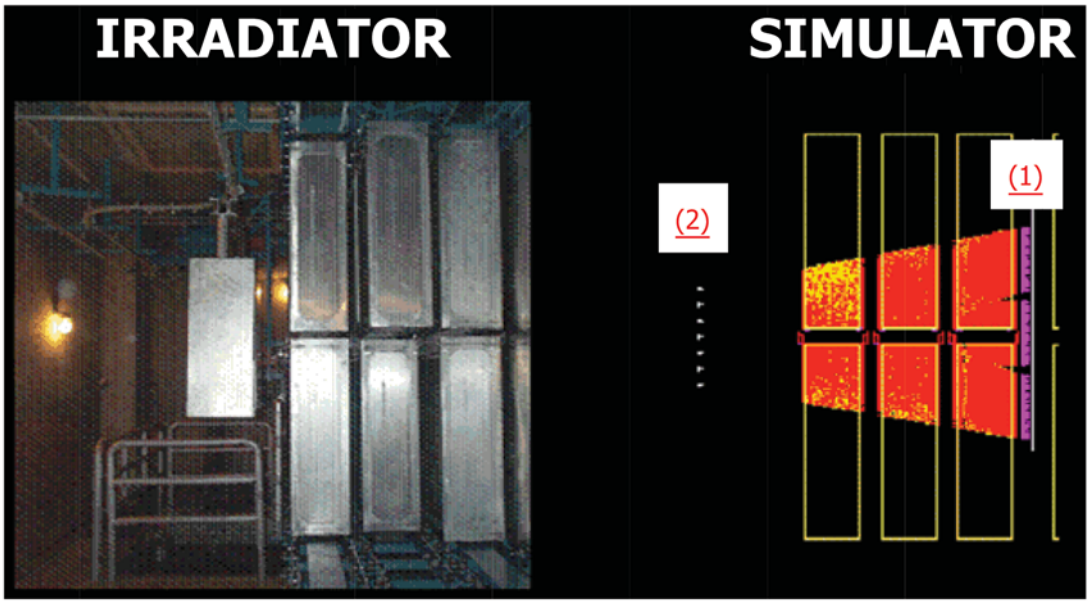

FIG. 2 Picture and Simulation of a Gamma Production Irradiator and Research Loop (36)

plans. The individual developing or using the selected model should be actively involved in the verification experiment(s). See Section 8 concerning the verification and validation experiments.

6.2.1 All training and significant experience of personnel involved in the modeling effort should be documented.

6.3 *Computer Equipment and Software*—Requirements should be reviewed and documented.

6.3.1 All significant pieces of hardware should be documented by name and, where appropriate, serial number.

6.3.2 All operating system software, modeling software, compilers and commercial products such as spreadsheets and data analysis tools should have their titles and version numbers recorded.

6.4 All relevant dosimetry data, reports of measurement and other physical evidence should be collected and filed or referenced for use in validation of model performance. See Section 8 concerning validation experiments.

7. Specification of Modeling Strategy and Method Selection

7.1 *Specification of the Modeling Effort*—All modeling approaches should be described in the form of a written protocol detailing the requirements for successful execution and subsequent completion of the exercise(s) relative to written criteria for success. The protocol should, at a minimum, include:

7.1.1 Specification of the source type and geometry as per 6.1.

7.1.2 Specification of facility (transport mechanism, support structures, biological shield as per 6.1).

7.1.3 Specification of target materials and geometries as per 6.1.

7.1.4 Declaration of personnel as per 6.2.

7.1.5 Specification of computer hardware and software as per 6.3 (see also 7.2).

7.2 *Criteria for Selection*—Most problems are rarely modeled exactly as they appear in reality; major approximations for simplification may be required to reduce the amount of effort required to build the model description and run times. These assumptions should be documented. Method selection will be primarily determined by the following criteria:

7.2.1 *Source Description*—For a photon source, any of the four methods may be chosen. For an electron source, the point kernel method is not recommended since the point kernel method assumes that the energy of the interacting particle is delivered at a point and then distributed statistically around that reaction point, as in the case of photons. On the other hand, electrons interact continuously with matter along their path and because of this the point kernel method is not appropriate.

7.2.2 *Level of Detail*—The level of detail to be included in the model, or the granularity of the problem, will influence the method selection. If the problem can be described as regions of homogeneous material, the point kernel method may be most appropriate if speed and spatial resolution are important. If the problem must be further broken down into smaller regions of different material (composition or density) in order to achieve accuracy, more complex input files will be needed.

7.2.2.1 Available software may have geometry replication and tiling features that are very useful for this purpose. If the target size is small relative to geometry or source description, Monte Carlo may require biasing or modification to include a larger volume wherein the dose will be an average value over a larger volume than desired. The Monte Carlo method can be used to provide a refinement of the point kernel build-up calculation to achieve the required accuracy with the point kernel method for optimized efficiency (time, resolution) (**27, 37, 38**).

7.2.3 *Set-up Time*—The complexity of three-dimensional problem descriptions in the input files and manipulation of the output files is where most of the effort is concentrated and can be very time consuming. It may also be necessary to make

modifications to the code to accommodate the specific problem to be solved. If modifications to the code are necessary, revalidation will be required, particularly if the physics modeled in the code has been changed.

7.3 *Selection of Method Type:*

7.3.1 The criteria for selection of a method type require input from various sources. Such sources include in-house and outside modeling expertise, model-based testing history and availability of verified and validated modeling code(s). These criteria should be documented as per 7.1.

7.3.2 Evaluation of the impact of the code on those items stated in 7.1.1 – 7.1.5 will typically be geared towards minimization of time for model set-up, execution and evaluation in exchange for exactness of solution set(s).

7.3.3 There are currently no written methods available for determining the optimum code to use. However, some general guidelines are as follows:

7.3.3.1 Empirical equations can be developed, evaluated against experimental results and, when found to satisfy written criteria within the limits established in the documentation, accepted and applied.

7.3.3.2 If empirical equations are unsatisfactory as determined by the user's criteria, deterministic or stochastic solutions, or both, may be sought.

NOTE 12—Deterministic or stochastic approaches, or both, may be utilized for the express purpose of supplementing a sparse measurement database so that empirical relationships can be established and employed.

NOTE 13—Because of the more rigorous physical models used in Monte Carlo codes, these may be considered for the purpose of verifying or validating performance of a proposed deterministic or empirical solution.

7.3.3.3 Various options are available to the end-user seeking deterministic or stochastic solutions, or both. Software packages related to these modeling techniques are listed in Annex A1. Refer to Table A3.1 in Annex A3 for guidance.

7.3.3.4 In all cases, validation of model performance should be done using a comprehensive measurement database (dosimetry results). See Section 8 concerning validation.

8. Verification and Validation of Model Performance

8.1 *Model Verification and Validation*—Validation compares the code output to results of an appropriate experiment. Verification confirms that the theory was implemented in a mathematically correct manner. Both verification and validation of a model require the use of a comprehensive measurement database of dosimetry results and other accepted calculations. In practice, verification and validation efforts often overlap during model testing.

8.1.1 *Model Benchmarking*—Model benchmarking is used both to verify a mathematical method and to validate the overall model construction and underlying physics of the method to produce reliable results. Comparing current model results with previously well-characterized systems is part of the model testing. Comparing model results with dosimetry for the specific problem being modeled is strongly recommended whenever possible. Differences between measurement and calculations should be consistent with uncertainty estimates for both the measurements and the calculations.

8.1.1.1 There are a limited number of referenced benchmark examples in the literature and these may be inadequate in number to validate a method and inadequate in detail for comparison with the model under consideration. The model of the application of interest should be as nearly the same as possible to the benchmark example. Benchmark examples may be found in Annex A5. An example comparing the results of several methods (Monte Carlo, deterministic and semi-empirical) with dosimetry can be found in Ref **(39)**.

NOTE 14—One or more well-defined problems may be run through the model on the user's hardware and software platform(s) and compared to accepted results for execution of the model generated by one or more organizations (typically, this includes, at a minimum, the firm issuing the modeling software). Input and output are compared, and the modeling package's performance is deemed verified upon successful completion of the test(s).

NOTE 15—Formal software testing is not addressed in this guide. It is desirable to perform calculations with a modeling code that has undergone a formal software validation program. The level of validation is commensurate with the application, and must be justified by the user. The intended use of software may also have GMP or ISO implications. Refer to Annex A2 for references and Guide E482 for further guidance on software validation. Validation of computer modeling software is a complex issue. In many cases, validation of all aspects of operation of the code under all proposed modeling conditions is not feasible. The user is advised of the possibility that none of the software packages referenced in Annex A1 may be validated to national or international standards. The user is also advised to compare the calculation results with the experimental results. If this is not possible it would be convenient to use, at least, two different computer-modeling codes.

8.2 *Particulars of Three-Dimensional Model Construction*—Procedures for building and using a three-dimensional model to integrate code results with dosimetry (verification) are discussed in Annex A5.

8.3 *Precautions and Implementation*—It is important to test all assumptions for validity and to compare the results against dosimetry whenever possible.

8.3.1 Dosimetry may be used to "fine tune" the model for the current system. This is an acceptable and recommended practice when performed by qualified personnel.

8.4 The verification and validation procedure should be adhered to and documented.

8.5 *Validation and Verification of New Computer Code Releases*—Revisions of mathematical models are intended to improve the physics or software functionality, or both. At a minimum, verification of output from the updated software with output from previously run input files should be performed.

9. Uncertainty in Model/Method Prediction

9.1 Similar to dosimetric measurement, an estimate of uncertainty should accompany dose calculations. As a minimum, accuracy of the calculated dose value may be expressed as the ratio of the calculated absorbed dose to the measured absorbed dose. The accepted degree of agreement between calculation and measurement will depend on the user's requirements.

9.1.1 Refer to 2.1 for ASTM standards on dosimetry methods and uncertainties and 2.4 for NIST Technical Note 1297 on uncertainties.

9.2 The Monte Carlo method does provide an estimate of the statistical uncertainty insofar as it relates to the calculation. The cross sections used in these calculations (and probably further hidden inside other types of calculations) will have usually published uncertainties which can be followed through via an uncertainty budget analysis.

9.3 Inadequate description of the problem and coding errors constitute a significant source of uncertainty. Biasing due to variation in geometry and composition of the irradiated products, and in the properties of the source are additional sources of uncertainty. Inherently, all models are approximations and limitations to geometry description and approximations to the actual physics will cause calculated values to differ. The distribution of these differences is typically unknown but is bounded by the validation and verification. Coding errors can cause both gross and subtle miscalculations.

9.4 Potential deficiencies in the application of mathematical models to problem solving include the following.

9.4.1 *Experience*—The methodology is excellent, but a mistake has been made in describing the input file (for example, geometry input). Error detection by software is generally limited to coding errors and cannot be relied upon to catch user errors that are embedded in formally correct code.

NOTE 16—Geometry validation packages are available for some radiation transport codes. They detect overlapping, ill coded regions and allow the visual verification of the geometry. Their use is highly recommended.

9.4.2 *Knowledge*—A good model is developed but the application is a failure.

9.4.2.1 *Discussion*—Examples of application failure are: running an insufficient number of histories when using a Monte Carlo code; dividing distances into too small an increment for the step size; and, using too high an energy cut-off or neglecting characteristic X-rays in thin multiple layers of different materials.

9.4.3 *Structural Support*—This may include software problems and hardware problems that are beyond the ability of the method to resolve.

9.4.3.1 *Discussion*—Limited ability of a 1-D code to match the number of layers in the problem forces combination of different materials, limited angle of incidence or inability to run Monte Carlo in adjoint mode.

9.4.4 *Other Factors Limiting Appropriate Benchmarking*—Ability to run dosimetry or lack of access to the problem; failure to perform a good measurement; lack of traceability or inability to perform dosimetry in critical elements of the problem.

9.4.5 *Information about the Problem*—Insufficient communication between the experimentalist and the model builder may obscure important details. Whenever possible, the model builder should be witness to the experiment and involved in all measurements.

10. Documentation

10.1 *General*—The following parameters, data and files should be stored for a defined duration. The records of each calculation should contain enough information to permit their repetition. These records include the identity of all personnel involved in the calculation. Ensure that all paper records and electronic records are properly protected.

10.2 *Input-Related Items:*

10.2.1 All relevant input parameters (files) should be included in the file associated with the results of execution of a modeling project.

10.2.2 *Relevant Model Description*—The calculation should reference a drawing or sketch illustrating the relevant details of the modelled design. For example, these details might include the type of irradiator and the type (or types) of radiation emitted by the radiation source, the radiation energy spectrum, including any filtration, the distance between the source and the surface or center of the irradiated specimen; physical data on the irradiated specimen (dimensions, mass, composition), characteristics of the container or apparatus used to hold the specimen during the irradiation and source geometry, including radionuclide distribution (if applicable).

10.2.3 *Relevant Computational Parameters*—Input parameters may also include but are not limited to such information as specified source distributions, subzone description, spatial mesh, discrete angles, energy cut-offs, and any non-default output options. The cross-section data for material composition should be available from the maximum source energy down to the chosen cutoffs for all materials defined in the problem geometry.

NOTE 17—If the gamma ray source energy spectrum incident on the specimen is not available, the information on the radiation source geometry (such as geometric shape of the source and cladding thickness) should be documented. For bremsstrahlung sources, the composition and thickness of the conversion target should be documented.

10.3 *Output-Related Items:*

10.3.1 All relevant input and output (files) should be included in the file associated with the results of execution of a modeling project.

10.3.2 *Relevant Diagnostic Output*—Examples of relevant output may include other results such as run time, energy conservation, charge conservation (where possible), statistical uncertainties and the number and energies of cascade particles generated (total and above cut-off).

10.3.3 Sufficient information (for example, title and version numbers for all operating system software, modeling software, compilers and commercial products such as spreadsheets and data analysis tools) should be stored so that if the problem is re-addressed, the original output from the problem can be compared to the output from the re-execution of said code.

10.4 *Post-Output Related Items*—The results of all post-output related processes (data manipulation, organization of results, etc.) should be recorded and filed according to accepted practices.

10.5 *Validation of Calculation Results with Dosimetry*—Whenever possible, the results of any set of calculations should be compared as directly as possible with dosimetry. These results should be recorded and filed with the input and output information. An error analysis should be performed to assess the relevance of any significant deviations. Any significant deviations should be addressed in the report.

10.6 *Additional Items to Document*—The experimental protocol used in generation and execution of the problem (see also 7.1). This should be referenced in all reports and related documentation.

10.6.1 References to all files associated with verification or validation, or both, of modeling software performance.

11. Keywords

11.1 benchmarking; deterministic method; discrete ordinates; empirical method; mathematical models; modeling; modelling; Monte Carlo; point kernel; radiation processing; radiation transport; stochastic; validation; verification

ANNEXES

(Informative)

A1. RADIATION MODELING CODES: SOURCES AND RELATED INFORMATION

A1.1 Monte Carlo codes including ITS, MCNP, EGS (EGSnrc) and PENELOPE point kernel codes including QAD-CGGP and coupled electron/photon discrete ordinates code CEPXS/ONELD and photon codes DANTSYS and TORT, and semi-empirical code EDMULT are available from RSICC (Radiation Safety Information Computational Center), Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States.[6] See A1.7 for source of ITS and other codes in Europe.

A1.1.1 More information on PENELOPE is available at The Nuclear Energy Agency (NEA), a specialized agency within the Organization for Economic Cooperation and Development (OECD) (http://www.oecd-nea.org/).

A1.2 The Monte Carlo code EGSnrc is available from the National Research Council of Canada, Ottawa. Refer to http://www.nrc-cnrc.gc.ca/eng/solutions/advisory/egsnrc-index.html.

A1.3 The Monte Carlo code MCBEND and point kernel code RANKERN are available from http://www.answerssoftwareservice.com/codes.html.

A1.4 The adjoint Monte Carlo code NOVICE is available from EMPC Experimental and Mathematical Physics Consultants. Refer to http://www.empc.com/novice.php.

A1.5 The TART Monte Carlo code is available from the Lawrence Livermore National Laboratory, (https://wci.llnl.gov/codes/tart/).

A1.6 A monthly newsletter is available from the RSICC detailing changes to the computer code and data library collection. The newsletter also provides a calendar and descriptions of future conferences, courses, workshops and symposia (https://rsicc.ornl.gov/RSICCNewsletters.aspx).

A1.7 The GEANT4 Monte Carlo code is available from CERN (https://gean4.web.cern.ch/gean4/index.shtml).

NOTE A1.1—The user should seek software-supplier guidance for minimum system operating requirements.

[6] For the complete online catalog, see https://rsicc.ornl.gov/Catalog.aspx?c=A-Z.

A2. REFERENCES FOR SOFTWARE VALIDATION

A2.1 General Principles of Software Validation; Final Guidance for Industry and FDA Staff, January 11, 2002 U.S. Department Of Health and Human Services Food and Drug Administration Center for Devices and Radiological Health Center for Biologics Evaluation and Research. Available at www.fda.gov.

A2.2 FDA Medical Device Quality System Manual, Design Control Guidance For Medical Device Manufacturers, March 1997. Available at www.fda.gov.

A2.3 IOS/IEC 90003, Software engineering—Guidelines for the application of ISO 9000:2008 to computer software. Available at www.iso.org.

A2.4 Software Quality Assurance—A Guide For Developers and Auditors, Howard T. Garston Smith, Available at CRC Press (www.crcpress.com).

A2.5 ANSI/IEEE Std 1012-98. IEEE Standard for Software Verification and Validation. IEEE, 345 East 47th Street, New York, NY, United States. Available at the IEEE Standards Association (http://standards.ieee.org).

A2.6 NIST Special Publication 500-234. Reference Information for the Software Verification and Validation Process. Available at www.NIST.gov.

A2.7 ANSI/IEEE Std 1012-98. IEEE Standard for Software Verification and Validation. IEEE, 345 East 47th Street, New York, NY, United States.

A2.8 NIST Special Publication 500–234. Reference Information for the Software Verification and Validation Process, USDOC, NIST, Gaithersburg, MD, United States, March 1996.

A3. PHYSICS AND MODELING TUTORIAL

NOTE A3.1—Several useful and well-known textbooks are available on the subjects of shielding (**26**) and transport methods (**40**).

A3.1 *Justification for Model Building*—In general, modeling of a process increases understanding and may lead to improved process efficiency. Modeling is particularly useful when the intended facility is not accessible due to design, location or scheduling. For electron beam processes, alternative product packaging designs may be considered to optimize dose uniformity, throughput and distribution of isotope activity/voltage selection. Modeling may be used to optimize a facility design in order to anticipate that a desired result is possible before committing time, resources and products to a potentially expensive experiment or fabrication. An example might be to develop a scheme for running materials of different densities in parallel, either as stratified layers within product or product conveyance structure, or sequentially in a series of product volumes.

A3.2 *Consideration of the Modeling Effort*—Radiation transport codes have been under development for several decades and have become quite sophisticated in their ability to solve problems. The parallel development of powerful, compact and inexpensive computers now makes their application both practical and accessible to a broad audience of users. The degree to which the various codes may mimic reality is commensurate with the complexity of the method and the effort applied in model building. Increasing the complexity of the system, the level of detail desired and the accuracy of the results will require more effort, experience, judgments and careful testing of the necessary simplifying assumptions. Some geometrically simple product forms such as flat sheet, tubing and wire can be accurately modeled. However, with complex product forms, assumptions are always made for simplification and speed but may compromise accuracy. Whenever possible, assumptions should be tested and verified. Level of experience will determine where to begin a modeling effort and a range of approaches is presented in this document. The novice is urged to use caution but should be aware that some approaches are simple and may be entirely adequate for the intended purpose. Unless trained personnel are available, an expert should be consulted before applying one of the more sophisticated approaches.

A3.3 *Brief Physics Tutorial*—If the background of the reader does not include any familiarity with radiation processing, this paragraph will be useful in understanding the content of this guide. The reader is referred to several useful articles on the physics of energy deposition and transport codes (**41**, **42**). Absorbed dose is a measure of the energy deposited per unit mass (refer to 2.3). Radiation deposits energy into matter by direct collision with electrons of the absorber and interactions are at an atomic level. This occurs by way of a number of processes detailed in the referenced texts. Photons have no charge or mass. Therefore, they can travel long paths before an interaction with an atom occurs. This is the reason that a source of photons such as ^{60}Co or ^{137}Cs or photons generated by electrons (X-radiation or bremsstrahlung) deposit energy over greater distances than electrons. Electrons, on the other hand, have charge and mass. Therefore, accelerated electrons have a high number of interactions per unit path length and, as a result, deposit their energy in a relatively short distance. The energy available is directly related to the accelerating voltage; therefore, higher energy electrons penetrate further into matter. Electrons are also scattered by their interactions with matter and may deposit a substantial amount of their energy at some distance from the primary track, particularly if they undergo a bremsstrahlung interaction so that a photon is generated, carrying energy a long way from the point of interaction. In addition, the scattering of electrons near boundaries between regions of different atomic number or density, or both, may not always be properly accounted for in some calculations, leading to over-or under-estimates of the doses in regions near these boundaries. Higher density matter will increase the electron interactions proportionately and the bremsstrahlung generated in this process will become more important as the atomic number (Z) of the material increases.

A3.4 *Method Selection*—This guide covers three basic types of methods ranging in complexity. At the simplest level these include empirical and semi-empirical methods that are easily applied. The deterministic methods, including point kernel, contain more physics and require more experience. The Monte Carlo method is stochastic and solves radiation transport problems from first principles and in true three dimensions. Software documentation is available but may be inadequate. Attending a course or workshop for a particular code is recommended for the less-experienced user. While there is no best approach, this guide is intended to help the user make an appropriate selection.

A3.4.1 *Cross-reference Table*—A summary of the considerations for choosing a mathematical method is shown in Table A3.1. The table provides only general guidance and the attributes listed are subjectively rated. The method selected strongly depends on the user's application.

A3.4.2 *Empirical and Semi-empirical Method*—The simplest approach is a model built on empirical methods, which may not rely on any computer codes at all. These types of models can be built from the results of dosimetry experiments. These models are confined to the boundaries of the experiments and a specific facility. They cannot be extrapolated beyond those limits. However, this may be entirely sufficient for the intended purpose. The simplest codes that are available are semi-empirical and they are relatively easy to use. In these methods, the physics has been parameterized and there is an ability to simulate changes in source energy, density and atomic number (Z). This allows making dose predictions where measurement is not possible but calculation results should always be confirmed and tested.

A3.4.3 *Deterministic Methods*—These methods solve a set of equations (Boltzmann) used to describe the physics of radiation transport (**22-25**). The calculations are often one-dimensional but have an angular and spatial distribution that permits dose mapping when projected into three-dimensional space. Point kernel methods are generally applied for this purpose. Because these methods are fast, great detail and fine resolution are possible in a reasonable amount of time. However, the solution of the Boltzmann equation, while exact, is valid for a given unit path length only and does not account for scattered radiation from the rest of the problem (three-dimension). There is no estimate provided for any error that this might introduce to the problem being described.

A3.4.4 *Monte Carlo Method*—This method is a three-dimensional method capable of including the radiation transport physics of the problem. These codes are sophisticated and reasonably mimic the real world. The model is sampled to provide a prediction with statistical uncertainty. A sample is a batch of particle histories that is only a small fraction of the real population of particles experienced in the actual world. As the sampling size increases, this method should converge with a higher level of precision. This is important for facility design and determining dose discontinuities at the boundaries of materials. The caveat is that the calculations take considerable computer time in order to get the desired precision. Some techniques exist within Monte Carlo to reduce the computational time. With some practice, these codes also may be fairly easily applied to solving one and even two-dimensional (for example, cylindrical geometry) systems. The use of this method for solving three-dimensional problems generally requires in-depth knowledge and judgment that can only come from experience.

A4. PARTICULARS OF THREE-DIMENSIONAL MODEL CONSTRUCTION

NOTE A4.1—The following tutorial is a general guide on how to build and use a three-dimensional model to integrate code results with dosimetry.

A4.1 *General*—The model should contain all elements of the geometry in question that will affect absorbed dose and dose distribution. Note that while it is necessary to include all the important components in detail, it is highly desirable from a practical viewpoint to simplify the description as much as possible. If the method permits modeling complex geometries, sensitivity calculations may be performed to justify some simplifications.

TABLE A3.1 Selection Matrix

Attribute	Monte Carlo	Point Kernel	Discrete Ordinates	Semi-Empirical	Empirical
Dimensional capability	3-D	3-D	3-D	N/A	N/A
Electrons	Yes	Rarely	Yes	Yes	Yes
Gamma, X-ray and Bremsstrahlung	Yes	Yes	Yes	Yes	Yes
Calculation Speed	Slow	Moderate	Slow[A]	Fast	Fast
Estimate of Precision	Yes	N/A	N/A	N/A	N/A
Resolution	Low	High	High	Moderate	N/A
Verification required	Yes	Yes	Yes	Yes	Yes
Available for Purchase	Yes	Yes	Yes	Yes	N/A

[A] Discrete ordinate methods are slower than the Monte Carlo method if one dose point is of interest, but can be faster for multiple dose points.

A4.1.1 The source of the radiation should be accurately described including its dimensions and energy. The geometry details of the irradiator should be accurately described using direct measurements or verification of physical drawings where applicable.

A4.1.2 Some simplification of elements may be necessary (cobalt sources, steel rollers) in order to reduce the number of input bodies. Care must be exercised to maintain mass and dimensions.

A4.1.3 Some methods permit simplification of a problem along axes of symmetry through the geometry by using a "mirror" to reflect radiation. This is sometimes known as albedo and the mirror effect can be accomplished by creating an albedo zone.

A4.1.4 The need to modify the model for the specific application may involve code modification, modifications to the geometry to include product movement into a time-independent code, and post-processing of output to get the results into a meaningful form for interpretation. Additional programming may be required for routine operation (for example, a user interface).

A4.1.5 After the simplifying assumptions are complete, there will be a minimum of 2 additional steps; model construction to include *(1)* homogeneous material, and *(2)* heterogeneous product. In both cases, dosimetry should be employed to validate both the model and the products. All such operations should be documented.

A4.2 *Photon Source Model Construction*:

A4.2.1 For a photon source the model could typically include such things as linear arrays of isotope, metal structural components and concrete walls that interact with the radiation environment sufficiently to affect the absorbed dose distribution in the product.

A4.2.2 A ^{60}Co gamma source will generally be described by its physical dimensions with a completely isotropic emission of two photons roughly having an equal probability. Note that due to physical geometries of radiation sources, an isotropic gamma radiation source may effectively become a non-isotropic source due to self-absorption, mutual absorption, source rack structure, and source encapsulation material.

A4.3 *Electron Source Model Construction*:

A4.3.1 For an electron beam, the model could typically include the titanium window foil, scan angles, distance from the product and metal components of the conveyor system, which might affect product dose. Modeling the effect of scattering structures to redirect a portion of the "escaping" electrons back towards the product may be evaluated.

A4.3.2 An electron beam source may be modeled as a distributed source, which is required in order to simulate product movement. The source description may consist of either a point or line origin with an isotropic distribution confined to one plane only and with a narrow angular distribution corresponding to the scan angle of the beam. The source particle energy in the case of electron beam will generally be the accelerating voltage and may be modified by the energy spectrum characteristics of a particular machine.

A4.4 *Product Movement (Conversion of Model Output into Dose)*—The various mathematical approaches for modeling a facility are generally time-independent and may require some modification in the geometry or adjustment to the dose calculation to accurately simulate the movement of product through the radiation field. This may not be necessary when using empirically derived parametric equations. In particular, this issue needs to be addressed for small, focused sources such as an electron beam.

A4.4.1 *Electron Beam*—Small or focused sources can be modeled as distributed sources so that the movement of the product through the radiation field can be accounted for **(43, 44)**.

A4.4.2 *Photon Source*—Large isotropic sources such as radioactive isotopes (^{60}Co) can usually be modeled as they actually appear and dose calculation will be a function of source strength and time.

A4.5 *Model of a Facility Using Homogeneous Product*—For validation of a facility, it may be convenient to use homogeneous product (for example, foam, cardboard, etc.) as the process load with dosimeters at specific locations. The model can then be based on a solid single homogeneous material to avoid excessive coding needed to describe heterogeneous product as an array of smaller bodies with different cross-sections. However, for real product, a homogeneous approximation is not always a safe assumption and dose mapping should always test the accuracy of the cross-sections.

A4.6 *Model of a Facility Using Specific Products*:

A4.6.1 For the product, the geometry would include detailed descriptions of the bodies broken down into components of density, composition and dimensions.

A4.6.2 The dimensions of the bodies through their association with density would describe objects. This may mean describing a packaged object by the location of the contents rather than by the package dimensions.

A4.6.3 Layered products (that is, sheets of material) may be sensitive with respect to orientation of an incident electron beam. When oriented parallel to the incident beam, the depth of penetration, magnitude and location of the backscatter maximum may be shifted deeper into the product.

A4.7 *Model of Dosimeters*:

A4.7.1 Homogeneous and heterogeneous products may be partitioned as individual zones or by subzones to define a dose map. The calculated result must be compared to a dosimetry measurement at specific locations within a specific product.

A4.7.2 In some cases the dosimeter may be a sufficiently large object such that it can be modeled directly. Precise location of a dosimeter in the product geometry is critical to achieving a valid comparison between the model calculation and the experimental measurement, especially when using an electron beam.

A4.7.3 In many cases the dosimeter may be too small to effectively model as an individual object in the full model description. This is a problem when using a Monte Carlo code because the object is very small and requires long run times in order to achieve adequate precision in the result. In these cases, a larger region within the product geometry description may be used to define a dosimeter by extending its thickness, area or mass density. The location of dosimeters should be mapped as regions to account for shifting/misalignment of dosimeters with actual location in the product geometry. This determines the dose sensitivity associated with placement of the dosimeter and allows determination of this source of uncertainty.

A4.7.4 Dose predictions must be validated by irradiating actual product with dosimeters in specific locations.

A4.8 *Dose Calculation*:

A4.8.1 For an electron beam model where the dose calculation is expressed as energy deposited per source electron per gram (E), the dose in the material in terms of the electron beam irradiation parameters can be obtained in the following way:

$$D = \frac{\bar{\epsilon}}{m} = \frac{E(\text{MeV} \quad \text{cm}^2/g \cdot e)N_e}{A(\text{cm}^2)}$$

with N_e, the number of electrons coming out of the accelerator and A the irradiation area in cm^2. These last two can be expressed in the following way:

$$N_e = \frac{I(\text{mA})\cdot t(\text{s})}{e(\text{mC})}$$

$$A(\text{cm}^2) = b(\text{cm})\cdot v(\text{cm}/s)\cdot t(s)$$

with I the beam current of the electron accelerator, t, the irradiation time and, bv the area processing rate. Also e is the charge of the electron in mC (1.6×10^{-16}mC). Using also the fact that 1 MeV/g=1.6×10^{-13} kGy, the dose in the material can be calculated as:

$$D(\text{kGy}) = 1000\frac{E_e(\text{MeV} \quad \text{cm}^2/g \cdot e)\cdot I(\text{mA})}{b(\text{cm})\cdot v(\text{cm}/s)}$$

NOTE A4.2—It may be important to remember that measured dose is in units of dose to water, which is often several percent different to the calculated dose to a non-water material. This may be accounted for using the average electron collisional stopping power ratio, which may be obtained for most materials using standard databases, for example, ESTAR at NIST (**45**).

A4.8.1.1 Suitable modifications to this simple equation may be required to adjust the calculation for movement of product through the radiation field.

A4.8.2 For a ^{60}Co gamma ray model where the dose calculation is expressed as energy deposited per photon per gram, the dose in the material in kGy can be obtained using the equations below:

$$D(\text{kGy}) = E_\gamma(\text{MeV}/g)N_\gamma = 2E_\gamma(\text{MeV}/g)S(\text{Bq})t(s)$$

where $N\gamma$ represents the number of gamma rays emitted by the radioactive source, which for ^{60}Co is equal to twice the activity of the source expressed in Bq (1 Ci=3.7×10^{10} Bq). Using also the conversion factor 1 MeV/g=1.6×10^{-13} kGy the dose will be:

$$D(\text{kGy}) = 3.2 \times 10^{-13}E_\gamma(\text{MeV}/g)\cdot S(\text{Bq})\cdot t(s)$$

NOTE A4.3—It may be important to remember that measured dose is in units of dose to water, which is often several percent different to the calculated dose to a non-water material. This may be accounted for using the average electron collisional stopping power ratio, which may be obtained for most materials using standard databases, for example, ESTAR at NIST, or by using the average mass-energy absorption coefficient, again from standard databases, for example, XCOM at NIST (**45**).

A5. BENCHMARKING

A5.1 *Code-to-code Comparison*—Compare code outputs against each other for the same geometry and sources. The same results should be obtained within uncertainty if the codes are installed correctly and are coded correctly (**46**). This reference effectively serves as a benchmark for several codes against each other.

A5.2 *Code-to-Dosimetry Comparison*—Use a real facility with traceable dosimetry and compare code results to actual measurement. Compare code output with reference-standard dosimetry system measurements. This is validation, that model building assumptions and approximations were correct in this reduction to practice (**47 and 48**).

A6. EXAMPLES OF DIFFERENT CODES

A6.1 *Examples for Monte Carlo Models*:

A6.1.1 Several general articles on Monte Carlo techniques and applications are cited in the references (**3, 20 and 21**) including the original article on condensed history Monte Carlo.

A6.1.2 A comparison between simple-geometry examples and more realistic examples of ETRAN Monte Carlo code can be found under "ETRAN—Experimental Benchmarks," and "Applications of ETRAN Monte Carlo Codes" of Ref (**40**).

A6.1.3 A comparison between simple and complex geometries for the ITS codes can be found in the various sections of "Applications of the ITS Codes" in Ref (**40**). A strategy for determining dose-depth relationships in standard construction geometries for a wide variety of applications using ITS can be found in Ref (**49**).

A6.1.4 An example of verification of a Monte Carlo code for thick target bremsstrahlung calculations can be found in Ref (**50**).

A6.1.5 Comparisons between Monte Carlo codes with regard to dosimetry at material interfaces, backscatter factors and depth-dose curves can be found in Refs (**36, 50**).

A6.1.6 Comparisons of dosimetry measurement with simulations of thin-layer slab geometry at low voltages of 100 to 300 keV, typical of radiation processing of web materials, can be found in Refs (**51, 52**). An example detailing dose and charge distribution relationships in sheet materials at electron voltages ranging from 0.4 to 10 MeV can be found in Ref (**53**).

A6.1.7 An example of modeling an electron beam source as an extended source to simulate product (tubing) movement, including sensitivity studies to justify model simplifications can be found in Ref (**43**). The same approach was later applied to other moving objects (bottles) in Ref (**44**). An example describing 3-D electron and X-ray dose distributions in water at 2 to 10 MeV with comparison with dosimetry at 2 MeV can be found in Ref (**54**).

A6.1.8 Several Monte Carlo gamma irradiation processing facility validation studies, including process planning and dose rate determinations, using MCNP can be found in Refs (**55-58**). These studies provide a good validation of the underlying physics and demonstrate the utility of using these models to evaluate facility design as well as routine and non-routine processing.

A6.1.9 An application of EGS4 for determination of gamma ray spectrum and dose rate distribution in a GammaCell 220 can be found in Ref (**42**).

A6.2 *Examples of Deterministic Models*:

A6.2.1 *Annotated Examples for the Discrete Ordinates Method:*

A6.2.1.1 Simple geometry one-dimensional and two-dimensional comparisons can be found in Ref (**39**).

A6.2.1.2 Forward and adjoint methods and applications can be found in Ref (**22**).

A6.2.1.3 A comprehensive comparison of CEPXS/ONELD calculations with the ^{60}Co data set of Wall and Burke can be found in Ref (**59**).

A6.2.1.4 A comparison of ONETRAN calculations with dosimetry measurement for ^{60}Co dose profile data to determine photon spectrum can be found in Ref (**60**).

A6.2.2 *Annotated Examples for the Point Kernel Method:*

A6.2.2.1 Annotated examples for the point kernel method can be found in Ref (**26**).

A6.2.2.2 A study of gamma ray buildup factors for a point isotropic source in stratified shields can be found in Ref (**38**).

A6.2.2.3 Early benchmark examples of models built using point kernel codes for ^{60}Co facilities, based on homogeneous materials, made predictions that were within 5 to 7 % of dosimetry (**4, 61**).

A6.2.2.4 Dose distribution predictions for a range of product densities have been mapped at high resolution (60 cm^3) to assess sterility assurance (**62**).

A6.2.2.5 Advanced examples of application of point kernel codes to industrial radiation processing (**37**), process control charting (**63**), "off-carrier" processing (**64**), and source rack loading planning (**65**) have recently appeared.

A6.3 *Examples of Semi-empirical Models*:

A6.3.1 *Annotated Examples for the Semi-empirical Method:*

A6.3.1.1 Extension of EDMULT code for calculation of dose distribution in tubing and coparison with dosimetry can be found in Ref (**50**).

A6.3.1.2 Semi-empirical method for depth-dose curves (**66**).

A6.3.1.3 EDMULT for 300 keV electron beam (**67**).

A6.3.1.4 Semi-empirical model for X-ray depth dose distribution, compared with Monte Carlo (**68**).

A6.3.1.5 Electron transmission energy distribution, empirical expression (**69**).

A6.4 *Additional Annotated Examples*—(**45, 70-108**)

REFERENCES

(1) Transpire Inc., www.transpireinc.com.

(2) Brynjolfsson, A., *Cobalt-60 Irradiator Designs: Sterilization by Ionizing Radiation—Volume 1*, Gaughran, E. R. L., and Goudie A. J., eds., Multiscience Publications Ltd., Montreal, Quebec, Canada, 1974, pp. 145-172.

(3) McIntyre, R., Huntzinger, C. J., and Nelson, W. R., "Applications of EGS4 to Industrial Irradiator Design and Use," *Radiat. Phys. Chem.*, 35 (4-6), 1990, pp. 762-766.

(4) Mosse, D. C., Laizier, J. J. M., Keraron, Y., Lallemant, T. F., and Perdriau, P. D. M., "Experimental Qualification of a Code for Optimizing Gamma Irradiation Facilities," *Radiat. Phys. Chem.*, 31 (4-6), 1988, pp. 555-562.

(5) Farrell, J. P., Seltzer, S. M. and Silverman, J., "Bremsstrahlung Generators for Radiation Processing," *Radiat. Phys. Chem.*, 22, 1983, pp. 469-478.

(6) Cleland, M. R., Thompson, C. C., Strelczyk, M., and Sloan, D. P., "Advances in X-ray Processing Technology," *Radiat. Phys. Chem.*, 35, 1990, pp. 632-637.

(7) Saylor, M. C., "Developments in Radiation Equipment Including the Application of Machine-Generated X-rays to Medical Product Sterilization," *Sterilization of Medical Products*, Volume V, Morrissey, R. F. and Prokopenko, Y. I., eds., Polyscience Publications Inc., Morin Heights, Canada, 1991, pp. 327-344.

(8) Seltzer, S. M., "An Overview of ETRAN Monte Carlo Methods," Jenkins, T. M., Nelson, W. R., and Rindi, A., (Eds.), "Monte Carlo Transport of Electrons and Photons," Plenum, New York, 1989, pp. 153-182.

(9) Seltzer, S. M., "Electron Photon Monte-Carlo Calculations: the ETRAN Code," *Appl. Radiat. Isot.*, 42, 1991, pp. 917-941.

(10) Halbleib, J. A., Kensek, R. P., and Valdez, G. D., "ITS: The Integrated TIGER Series of Electron Photon Transport Codes: Version 3.1," *IEEE Trans. Nuc. Sci.*, 39, 1992, pp. 1025-1030.

(11) Halbleib, J. A., Kensek, R. P., Mehlhorn, T. A., Valdez, G. D., Seltzer, S. M., and Berger, M. J., *ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes*, SAND91-1634, Sandia National Laboratories, 1992.

(12) Lorence, L. J., Kensek, R. P., Halbleib, J. A., and Morel, J. E., "Adjoint Electron-Photon Transport Monte Carlo Calculations with ITS," *IEEE Trans. Nuc. Sci.*, 42, 1995, pp. 1895-1901.

(13) Smith, L. M., and Hochstedler, R. D., "Accelerating Execution of the Integrated TIGER Series Monte Carlo Radiation Transport Codes," *IEEE Trans. Nuc. Sci.*, 44, 1997, pp. 36-41.

(14) Kensek, R. P., Halbleib, J. A., and Valdez, G. D., "ITS–Some Practical Advice," *Trans. Am. Nuc. Soc.*, 73, 1995, pp. 330-331.

(15) Nelson, W. R., Hirayama, H., and Rogers, D. W. D., *The EGS4 Code System*, Stanford Linear Accelerator Center Report SLAC-265, 1985.

(16) Breismeister, J. F., ed., *MCNP–A General Monte Carlo N-Particle Transport Code, Version 4C*, LA-13709-M, Los Alamos National Laboratory, Los Alamos, New Mexico, April 2000 .

(17) Baro, J., Sempau, J., Fernandez-Varea, J. M., and Salvat, F., "PENELOPE: An Algorithm for Monte-Carlo Simulation of the Penetration and Energy-Loss of Electrons and Positrons in Matter," *Nucl. Instr. Meth.*, B100, 1995, pp. 31-46.

(18) Cox, L. J., Schach von Wittenau, A. E., Bergstrom Jr., P. M., Mohan, R., Libby, B., Wu, Q., and Lovelock, D. M. J., "Photon Beam Description in PEREGRINE for Monte Carlo Dose Calculations," Lawrence Livermore National Laboratory, UCRL-JC-126731, 1997.

(19) Bielajew, A. F., and Rogers, D. W. O., "PRESTA: The Parameter Reduced Electron Step Transport Algorithm for Electron Monte Carlo Transport," *Nucl. Instr. Meth.*, B 18, 1987, pp. 165-181.

(20) Salvat, F., Fernandez-Varea, J. M., Sempau, J., and Mazurier, J., "Practical Aspects of Monte Carlo Simulation of Charged Particle Transport: Mixed Algorithms and Variance Reduction Techniques," *Radiat. Environ. Biophys.*, 38, 1999, pp. 15-22.

(21) Nahum, A. E., "Condensed History Monte Carlo Simulation for Charged Particles: What Can It Do For Us?," *Radiat. Environ. Biophys.*, 38, 1999, pp. 163-173.

(22) Drumm, C. R., Fan, W. C., and Renken, J. H., "Forward and Adjoint Methods and Applications for Deterministic Electron-Photon Transport," *Nucl. Sci. Engin.*, 108, 1991, pp. 16-49.

(23) Lorence, L. J., Nelson, W. E., and Morel, J. E., "Coupled Electron-Photon Transport Calculations Using the Method of Discrete Ordinates," *IEEE Trans. Nuc. Sci.*, 32, 1985, pp. 4416-4420.

(24) Duderstadt, J. J., and Martin, W. R., "Transport Theory," Wiley Interscience, New York, 1979.

(25) Drumm, C. R., "Multidimensional Electron-Photon Transport with Standard Discrete Ordinates Codes," *Nucl. Sci. Engin.* 127, 1997, pp. 1-21.

(26) Shultis, J. K., and Faw, R. E., *Radiation Shielding*, Prentice-Hall PTR., Upper Saddle River, NJ, 1996.

(27) Carter, L. L., Morford, R. J., Frederickson, S. M., and Hillesland, K., *Point Kernel Option in MCNP at the Hanford Site*, Proceedings for 8th International Conference on Radiation Shielding at Arlington, Texas, April 1994.

(28) Tabata, T., Andreo, P., and Shinoda, K., "An Analytic Formula for the Extrapolated Range of Electrons in Condensed Materials," *Nucl. Instr. Meth.*, B119, 1996, pp. 463-470.

(29) Tan, D., and Heaton, B., "Simple Empirical Relations for Electron CSDA Range and Electron Energy Loss," *Appl. Radiat. Isot.*, 45, 1994, pp. 527-528.

(30) Tabata, T., and Andreo, P., "A Method to Convert Absolute Depth-Dose Curves of Electrons Between Different Phantom Materials," *Jap. J. Med. Phys.*, 17, 1997, pp. 151-160.

(31) Tabata, T., and Ito, R., "An Algorithm for Electron Depth-Dose Distributions in Multilayer Slab Absorbers," *Jap. J. Appl. Phys.*, 20, 1981, pp. 249-258.

(32) Tabata, T., Ito, R., and Tsukui, S., "Simple Method of Evaluating Absorbed Dose in Electron-Beam Processing," *Radiat. Phys. Chem.* 33, 1989, pp. 411-416.

(33) Tabata, T., "Semiempirical Models for Depth-Dose Curves of Electrons in Matter: An Introductory Review," *Bull. Univ. Osaka Prefect.*, 41, 1993, pp. 103-118.

(34) Tabata, T., "Theoretical Evaluation of Absorbed Doses in Materials Irradiated by Low-Energy Electron Beams: A Short Review," *Bull. Univ. Osaka Prefect.*, 44, 1995, pp. 41-46.

(35) Illustration provided by Mark Bailey (personal communication), October 2016.

(36) Radiation Process Radiation Process Simulation and Modeling User Group (RPSMUG), www.rpsmug.org.

(37) Saylor, M. C., and Jordan, T. M., "Application of Mathematical Modeling Technologies to Industrial Radiation Processing," *Radiat. Phys. Chem.*, 57, 2000, p. 697.

(38) Lin, U. T., and Jiang, S. H., "A Dedicated Empirical Formula for G-Ray Buildup Factors for a Point Isotropic Source in Stratified Shields," *Radiat. Phys. Chem.*, 48, 1996, p. 389.

(39) Zhou, Y., Zhou, Y. Y., and Luo, Z. M., "Measurements and Calculations of Absorbed Dose in Electron Beam Radiation Processing," *Radiat. Phys. Chem.*, 42, 1993, pp. 817-820.

(40) Jenkins, T. M., Nelson, W. R., and Rindi, A., eds., *Monte Carlo Transport of Electrons and Photons*, Plenum Press, New York, 1988.

(41) Seltzer, S. M., "Physics of ETRAN and ITS Electron-Photon Monte Carlo Codes," *Trans. Am. Nuc. Soc.*, 73, 1995, pp. 332-333.

(42) Raisali, G. R., and Sohrabpour, M., "Application of EGS4 Computer Code for Determination of Gamma Ray Spectrum and Dose Rate Distribution in Gammacell 220," *Radiat. Phys. Chem.*, 42 (4-6), 1993, pp. 799-805.

(43) Weiss, D. E., Johnson, W. A., and Kensek, R. P., "Dose Distributions in Tubing: Monte Carlo Simulation and Measurement," *Radiation Physics and Chemistry*, 50, 1997, pp. 475-485.

(44) Weiss, D. E., Cleghorn, D. A., and Nablo, S. V., "Electron Beam Process Validation for Sterilization of Complex Geometries," *Radiat. Phys. Chem*., 2002, Vol. 63, pp 581–586.

(45) See for example: http://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html.

(46) Oliveira, A. D. and Oliveira, C., "Comparison of deterministic and Monte Carlo methods in shielding design," *Radiat. Prot. Dosim*., 115, 2005, pp. 254-257.

(47) Amako, K., Guatelli, S., Icanchenko,V. N., Maire, M., Mascialino, B., Murakami, K. I., Nieminen, P., Pandola, L., Parlati, S., Pia, M. G., Piergentili, M., Sasakik, T., Urban, L., "Comparison of Geant4 electromagnetic physics models against the NIST reference data," *IEEE Trans Nuc Sci*. 52, 2005, pp. 910-918.

(48) Cramer, S. N., "Analytic radiation transport systems and Monte Carlo benchmarks," *Nucl. Sci. Engin*. 139, 2001, pp. 186-208.

(49) Floyd, J. E., and Chappas, W. J., "Dose-Depth Simulations in Standard Construction Geometries," *Radiat. Phys. Chem*., 48, No. 2, 1996, pp. 179-194.

(50) Zhou, Y., Zhou, X., An, Z., Zhou, Y., and Wang, S., "Measurements and Calculations of Electron Dose Distributions in Circular Materials," *Radiat. Phys. Chem*., 63, 2002, pp. 723-727.

(51) Kojima, T., and Nakase, Y., "Electron-Beam Dosimetry for a Thin-Layer Absorber Irradiated by 300-keV Electrons," *Appl. Radiat. Isot*., 44, 1993, pp. 693-699.

(52) Kojima, T., and Nakase, Y., "Monte-Carlo Calculations of the Behavior of 300 keV Electron from Accelerators," *Radiat. Measurements*, 26, 1996, pp. 159-168.

(53) Cleland, M., Galloway, R., Genin, F., and Lindholm, M., "The Use of Dose and Charge Distributions in Electron Beam Processing," *Radiat. Phys. Chem*., 2002, Vol. 63, pp 729–733.

(54) Ziaie, F., Zimek, Z., Bulka, S., Afarideh, H., and Hadji-Saeid, S. M., "Calculated and Measured Dose Distribution in Electron and X-ray Irradiated Water Phantom," *Radiat. Phys. Chem*., 63, 2002, pp. 177-183.

(55) Oliveira, C., Salgado, J., Botelho, M. L. and Ferreira, L. M., "Dose Determination by Monte Carlo–A Useful Tool in Gamma Radiation Process," *Radiat. Phys. Chem*., 57, 2000, pp. 667-670.

(56) Oliveira, C., Salgado, J., and Carvalho, A. F., "Dose Rate Determinations in the Portuguese Gamma Irradiation Facility: Monte Carlo Simulation and Measurements," *Radiat. Phys. Chem*., 58, 2000, pp. 279-285.

(57) Oliveira, C., Ferreira, L. M., Goncalves, I. F., and Salgado, J., "Monte Carlo Studies of the Irradiator Geometry of the Portuguese Gamma Irradiation Facility," *Radiat. Phys. Chem*., 2002, Vol. 65, pp 293–295.

(58) Sohrabpour, M., Hassanzadeh, M., Shahriari, M., and Sharifzadeh, M., "Dose Distribution of the IR-136 Irradiator Using a Monte Carlo Code and Comparison with Dosimetry," *Radiat. Phys. Chem*., 2002, Vol. 63, pp 769–772.

(59) Garth, J. C., Critchfield, K. L., Turinetti, J. R., and Beutler, D. E., "A Comprehensive Comparison of CEPXS/ONELD Calculations of Dose Enhancement with the Co-60 Data Set of Wall and Burke," *IEEE Trans. Nuc. Sci*., 43, 1996, pp. 2731-2741.

(60) Woolf, S., and Garth, J. C., "Comparison of ONETRAN Calculations with Co-60 Dose Profile Data to Determine the Photon Spectrum," *IEEE Trans. Nuc. Sci*., 33, 1986, pp. 1252-1257.

(61) Cleland, M. R. et al, "Comparisons of Monte Carlo and ICRU electron energy vs range equations, *Radiat. Phys. Chem*, 2004, 71, pp. 585-589.

(62) Chu, R. D. H., and Vandyk, G. G., "The Effect of Dose Distribution on Sterility Assurance for Gamma Sterilized Medical Products," *Radiat. Phys. Chem*., 42, 1993, p. 585.

(63) Saylor, M. C., Connaghan, J. P., Yeadon, S. C., Herring, C. M., and Jordan, T. M., "Design and Application of Process Control Charting Methodologies to Gamma Irradiation Practices," *Radiat. Phys. Chem*., 2002, pp. 621-626.

(64) Baryschpolec, L. M., Wade, D. M., Herring, C. M., and Saylor, M. C., "Application of Mathematical Modeling-Based Algorithms to "Off-Carrier" Cobalt-60 Irradiation Processes," *Radiat. Phys. Chem*., 2002, 73-76.

(65) Pyne, C. H., and Comben, M. J., "Use of Validation Dosimetry, in Source Rack Load Planning, to Improve Cobalt Irradiation Plant Efficiency," *Radiat. Phys. Chem*., 2002, Vol 63, pp 785–788.

(66) Vazquez-Polo, G. et al, "Calculation of absorbed dose of low-energy electron beam by an approximate method," *Radiat. Phys. Chem*, 64, 2002, pp. 181-187.

(67) Hakoda, T. et al, "Absorbed dose rate distribution in 300 keV electron beam irradiation field for waste-gas purification," *Radioisotopes*, 53, 2004, pp. 59-69.

(68) Miller, R. B., "Food irradiation using bremsstrahlung x-rays," *Radiat. Phys. Chem*., 68, 2003, pp. 963-974.

(69) Staub, P. F., "The energy distribution of an electron beam transmitted through a solid film: a search for an empirically founded analytic expression," *J. Phys. D*, 28, 1995, pp. 252-257.

(70) Connaghan, J. P. et al, "Mathematical modeling of industrial radiation processes. Application and end-user training," *Radiat. Phys. Chem*, 71, 2004, pp. 335-338.

(71) Molinari, V. G., Manservisi, S., Rocchi, F., and Teodori, F., "Modeling of radiation transport," *Nucl. Instr. Meth*., B213, 2004, pp. 75-81.

(72) Michieli, I., "Point kernel calculation of dose fields from line sources using expanded polynomial form of buildup factor data: generalized secant integral-series representation," *Radiat. Phys. Chem*., 51, 1998, pp. 121-128.

(73) Tombakoglu, M., "An analytical solution to simplified photon transport model used for code verification," *Nucl. Instr. Meth*., B244, 2006, pp. 343-348.

(74) Allison, J., Agostineli, S., et al, "GEANT4- a simulation toolkit," *Nucl Instr Methods in Physics Research*, A 506, 2003, pp. 250-303.

(75) Bielajew, A. F. and Salvat, F., "Improved electron transport mechanics in the PENELOPE Monte-Carlo model," *Nucl. Instr. Meth*., B 173, 2001, pp. 332-343.

(76) Ravat, B. et al, "Energetic distribution of the electrons from a 200 keV beam in polyurethane layers: EGS4 calculation and FTIR analysis," *Radiat. Phys. Chem*, 61, 2001, pp. 571-573.

(77) Kaluska, I. and Popov, G. F., et al, "Basic Laws of boundaries effects for the absorbed dose distribution of electrons in the heterogeneous materials," Bulletin of the Kharkiv National University, 619, 2004, pp. 65-76.

(78) Cho, S. H. et al, "Validity of two simple rescaling methods for electron/beta dose point kernels in heterogeneous source-target geometry," *Radiat. Phys. Chem*, 69, 2004, pp. 265-272.

(79) Stichelbaut, F. et al, "X-ray dosimetry: comparing Monte Carlo simulations and experimental data," *Radiat. Phys. Chem*, 2004, pp. 345-349.

(80) Salvat, F. et al, "Monte Carlo simulation of bremsstrahlung emission by electrons," *Radiat. Prot. Dosim*, 116, 2005, pp. 113-117.

(81) Mohamed, A. B., Silverman, J., Weiss, D. E., and Al-Sheikhly, M., "Monte Carlo simulations of complex geometries and an optimal 60 Cobalt source design using the integrated TIGER series (ITS 3.0)," *Nucl. Instr. Meth*., B243, 2006, pp. 359-370.

(82) Legarda, F. and Idoeta, R. "Monte Carlo transport of electrons and positrons through thin foils," *Radiat. Phys. Chem*, 61, 2001, pp. 549-551.

(83) Van Laere, K. and Mondelaers, W. "Full Monte Carlo simulation and optimization of a high-power bremsstrahlung converter," *Radiat. Phys. Chem*, 49, 1997, pp. 207-219.

(84) Gharbi, F., Kadri, O., Farah, K. and Mannai, K. "Validation of GEANT code of CERN as predictive tool of dose rate measurement in the Tunisian gamma irradiation facility," *Radiat. Phys. Chem*, 74, 2005, pp. 102-110.

(85) Fragoso, M., Seco, J., Nahum, A.E., and Verhaegen, F., "Incorporation of a combinatorial geometry package and improved scoring

capabilities in the EGSnrc Monte Carlo Code system," *Med. Phys*., 30, 2003, pp. 1076-1085.
(86) Salvat, F., Llovet, X., Campos, C., Segui, S., Acosta, E., Fernandez-Varea, J. M., and Sempau, J., "Review of recent work using the simulation code PENELOPE," Application of Accelerators in Research and Industry: 17th Int'l Conference, Duggan, J. L., Morgan, I. L., eds, American Institute of Physics, 2003.
(87) Sempau, J., Fernandez-Varea, J. M., Acosta, E., and Salvat, F., "Experimental benchmarks of the Monte Carlo code PENELOPE," *Nucl. Instr. Meth*., B207, 2003, pp. 107-123.
(88) Forster, R. A., Cox, L. J., Barrrett, R. F., Booth, T. E., Briesmeister, J. F., Brown, F. B., Bull, J. S., Geisler, G. C., Goorley, J .T., and Mosteller, R. D., "MCNP version 5," *Nucl. Instr. Meth*., B213, 2004, pp. 82-86.
(89) Kijima, T., Kotera, M., Suga, H., and Nakase, Y., "Monte-Carlo calculations on the passage of electrons through thin-films irradiated by 300 keV electrons," IEICE Tr Electronics E78C, 1995, pp. 557-563.
(90) Meissner, J., Abs, M., Cleland, M. R., Herer, A. S., Jongen, Y., Kuntz, F., and Strasser, A., "X-ray treatment at 5 MeV and above," *Radiat. Phys. Chem*., 57, 2000, pp. 647-651.
(91) Borglund, N., Eriksson, J., Fumero, E., Kjall, P., Martensson, L., Orsholm, C., and Sikora, T., "Geometry package for Monte Carlo simulations," *Nucl. Instr. Meth*., A525, 2004, pp. 417-420.
(92) Gabler, D., Henniger, J., and Reichelt, U., "AMOS–An effective tool for adjoint Monte Carlo photon transport," *Nucl. Instr. Meth*., B251, 2006, pp. 326-332.
(93) Salvat, F., Fernández-Varea, J. M., and Sempau, J., "PENELOPE-2006, A Code System for Monte Carlo Simulation of Electron and Photon Transport," Workshop Proceedings, Barcelona, Spain, 4-7 July 2006, NEA 6222.
(94) Kaluska, I., Lazurik, V. T., Lazurik, V. M., Popov, G. F., Rogov, Yu. V., and Zimek, Z., "Dose distribution in the heterogeneous materials irradiated by electron beams," Institute of Nuclear Chemistry and Technology, INCT, Warsaw, Poland. Available from popov@univer.kharkov.ua.
(95) Kaluska, I., Lazurik, V. T., Lazurik, V. M., Popov, G. F., Rogov, Yu. V., and Zimek, Z. "Basic laws of boundaries effects for the absorbed dose distribution of electrons in the heterogeneous materials," Institute of Nuclear Chemistry and Technology, Warsaw, Poland. Available from popov@univer.kharkov.ua.
(96) Lazurik, V. T., Lazurik, V. M., Popov, G. F., and Rogov, Yu. V., "Simulation methods for quality control of radiation technologies," Available from popov@univer.kharkov.ua.
(97) Lazurik, V. T., Lazurik, V. M., Popov, G. F., and Rogov, Yu. V., "RT-Office for optimization of industrial EB and X-ray processing," Kharkov National University, Kharkov, Ukraine E-mail: popov@univer.kharkov.ua.
(98) Castanier, E., Kerouanton, D., "Evaluating the Gamma Dose Rate for the Liquid Waste Treatment Facility with Attila Radiation Transport Code," ICRS-12 & RPSD-2012 Conference Proceedings, Sept. 2-7, 2012, Nara, Japan.
(99) Wareing, T., McGhee, J., Barnett, A., Failla, G., and Davis, I., "Capabilities of Attila for Radiation Protection and Shielding," invited paper presented at the American Nuclear Society Winter Meeting, Albuquerque, NJ, November 12-16, 2006.
(100) Wareing, T., Horton, J., Mourtada, F., McGhee, J., Barnett, D., Failla, G., and Mohan, R., "Investigation of a Deterministic Method Incorporating Coupled Photon-Electron Transport for Photon Beam Dose Calculations in the Presence of Heterogeneities," AAPM Annual Meeting, Pittsburg, PA., 2004, pp. 821-825.
(101) Review of Monte Carlo Modelling Codes, The Panel on Gamma and Electron Irradiation Modelling Working Group, The Irradiation Panel, May, 2007, Revised January 2010.
(102) Bailey, M., Sephton, J., Sharpe, P., "Monte Carlo Modelling and Real-Time Dosemeter Measurements of Dose Rate Distribution at a ^{60}Co Industrial Irradiation Plant," *Radiat. Phys. Chem.*., 78, 2009, pp. 452-456.
(103) Sephton, J. P., Sharpe, P. H. G, Chu, R. D. H., O'Hara, K. P. J., Abdel-Rehim, F., Abdel Fattah, A., "Dose Mapping of a ^{60}Co Industrial Irradiation Plant Using an Electronic Data Recording System, Static Measurements and Mathematical Modeling," *Radiat. Phys.Chem.*, 76, 2007, pp. 1820-1825.
(104) Miller, A., "Uncertainty of Dose Measurement in Radiation Processing," *Radiat. Phys. Chem*., 47, 1996, p. 479.
(105) Whittaker, B., "Uncertainties in Absorbed Dose as Measured Using PMMA Dosimeters," *Radiat. Phys. Chem*., 42, 1993, pp. 841-844.
(106) Demarco, J. J., Solberg, T. D., Wallace, R. E., and Smathers, J. B., "Verification of the Monte Carlo Code MCNP for Thick Target Bremsstrahlung Calculations," *Med. Phys*., 22, 1995, pp. 11-16.
(107) Juste, B., Miro, R., Campayo, J. M., et al., "Comparison of Experimental 3D Dose Curves in a Heterogeneous Phantom," *Appl. Radiat. Isot*., 68, 2010, pp. 913-917.
(108) Sidlova, V., Trojek, T., "Testing Monte Carlo Computer Codes for Simulation of Electron Transport in Matter," *Appl. Radiat. Isot*., 68, 2010, pp. 961-964.