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

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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 determine the effectiveness of the radiation process, estimate the absorbed-dose distribution in product, or supplement and/or complement dosimetry measurements.

1.2 Radiation processing is an evolving field and annotated examples are provided in Annex A4 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 in the energy range of 0.1 to 25 MeV.

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

1.5 General purpose software packages are available for the calculation of the transport of charged and/or neutral particles and photons 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, energetic electrons from particle accelerators, or bremsstrahlung 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.

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:*

E 170 Terminology Relating to Radiation Measurements and Dosimetry[2]

E 482 Guide for Application of Neutron Transport Methods for Reactor Vessel Surveillance[2]

E 666 Practice for Calculating Absorbed Dose from Gamma or X Radiation[2]

2.2 *ISO/ASTM Standards:*

51204 Practice for Dosimetry in Gamma Irradiation Facilities for Food Processing[2]

51275 Practice for Use of a Radiochromic Film Dosimetry System[2]

51400 Practice for Characterization and Performance of a High-Dose Radiation Dosimetry Calibration Laboratory[2]

51431 Practice for Dosimetry in Electron and Bremsstrahlung Irradiation Facilities for Food Processing[2]

51608 Practice for Dosimetry in an X-ray (Bremsstrahlung) Facility for Radiation Processing[2]

51649 Practice for Dosimetry in an Electron Beam Facility for Radiation Processing at Energies between 300 keV and 25 MeV[2]

51702 Practice for Dosimetry in a Gamma Irradiation Facility for Radiation Processing[2]

51707 Guide for Estimating Uncertainties in Dosimetry for Radiation Processing[2]

51818 Practice for Dosimetry in an Electron Beam Facility for Radiation Processing at Energies between 80 and 300 keV[2]

51939 Practice for Blood Irradiation Dosimetry[2]

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

ICRU Report 14, Radiation Dosimetry: X-Rays and Gamma

[1] This guide is under the jurisdiction of ASTM Committee E10 on Nuclear Technology and Applications and is the direct responsibility of Subcommittee E10.01 on Dosimetry for Radiation Processing.

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[2] *Annual Book of ASTM Standards*, Vol 12.02.

[3] Available from International Commission on Radiation Units and Measurements, 7910 Woodmont Ave., Suite 800, Bethesda, MD 20814 USA.

Rays with Maximum Photon Energies Between 0.6 and 50 MeV

ICRU Report 17, Radiation Dosimetry: X-Rays Generated at Potentials of 5 to 150 kV

ICRU Report 34, The Dosimetry of Pulsed Radiation

ICRU Report 35, Radiation Dosimetry: Electron Beams with Energies Between 1 and 50 MeV

ICRU Report 37, Stopping Powers for Electrons and Positrons

ICRU Report 51, Quantities and Units in Radiation Protection Dosimetry

ICRU Report 60, Fundamental Quantities and Units for Ionizing Radiation, 1998

2.4 *International Organization for Standardization:*[4]

ISO 9001 Quality Systems—Model for Quality Assurance in Design/Development, Production, Installation and Servicing

ISO 9002 Quality Systems—Model for Quality Assurance in Production and Installation

ISO 11137 Sterilization of Health Care Products—Requirements for Validation and Routine Control - Radiation Sterilization

3. Terminology

3.1 *Definitions:*

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

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

3.1.2.1 *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.

3.1.3 *build-up factor*—the ratio of the total dose, particle fluence, exposure or other quantity due to primary and secondary (scattered) radiation, at a target (or field point) location to the dose due to primary radiation at that location. The concept of build-up applies to the transport of photons.

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

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

3.1.5 *discrete ordinates*—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.

3.1.5.1 *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 beam sources when appropriate assumptions can be made.

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

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

3.1.7 *histories*—a particle history is the record of all simulated interactions along its track as used in stochastic or Monte Carlo simulations.

3.1.7.1 *Discussion*—A 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.

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

3.1.9 *mathematical model*—a mathematical description of a physical problem based on physical laws and/or empirical correlation.

3.1.10 *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. 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.

3.1.10.1 *Discussion*—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*.

[4] Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036 USA.

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

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

3.1.11.1 *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).

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

3.1.12.1 *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, 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.

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

3.1.14 *radiation transport theory*—an analytical description of the propagation of a radiation field according to the physical laws governing the interactions of the radiation.

3.1.14.1 *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.

3.1.15 *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.

3.1.15.1 *Discussion*—The satisfaction of such physical rules may enable the model to be applicable over a wide range of energies and materials. A good example of a semi-empirical model for electron beam energy deposition is found in reference **(2)**.

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

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

3.1.18 *transport equation*—an integrodifferential equation describing the motion of particles or radiation through a medium. This equation contains various terms corresponding to sources of particles, particle streaming and particle scattering in and out of an infinitesimal volume of phase space.

3.1.19 *uncertainty*—a parameter associated with the result of a measurement, that characterises the spread of values that could reasonably be attributed to the measurand or derived quantity.

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

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

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

3.1.21.1 *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 cutoff 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.

3.1.22 *zoning*—The geometric description used to break up a larger region into smaller segments in which to calculate the dose. 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 E 170. Definitions in Terminology E 170 are compatible with ICRU 51 and 60; 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 references **(3-9)**.

4.7 *Validation*—The validation of model performance 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. See discussion under definition in Section 3 of this document.

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). In many cases, 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 A4 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 dose delivered 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 models are in use: Monte Carlo, deterministic, semi-empirical and empirical. Both Monte Carlo and deterministic models are based on the detailed physics of the interaction of radiation with matter.

5.2.1 Monte Carlo methods involve simulating paths of individual particles (either photons or electrons) and estimating dose by summing and averaging the histories of many particles.

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 target. See Note 1, references **(10-23)** and Annex A1 for examples and codes.

5.3.1 *Advantages*—Unlike other methods, the Monte Carlo method can theoretically account for all particle interactions and provide a faithful and accurate simulation of actual events. All contributions to the absorbed dose can be taken into account including scatter events in nearby objects. The Monte Carlo method is the method most capable of simulating the actual radiation transport in complex three-dimensional geometry.

5.3.2 *Disadvantages*—Depending on the quantity being calculated, Monte Carlo calculations tend to require execution times that are longer than deterministic methods to obtain satisfactory precision of dose estimates. In practice, exact simulation of all photon and electron paths is not feasible, so approximations and/or variance reduction techniques must be employed. For electrons, approximate trajectories using large path length steps and a multiple-scattering approach to particle deflections are used in standard Monte Carlo codes (See Annex A1). Such approximate paths may lead to significant errors, particularly when transport across surfaces or material interfaces is important.

NOTE 2—To minimize computation 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 greatest 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 target size is small relative to geometry or source description, Monte Carlo calculations may require extra long run times, biasing or modification to include a target volume wherein the dose will be an average value over a larger volume than desired. This type of problem may occur when attempting to calculate the dose at dosimeters with small volume.

5.3.2.3 Calculations of dose should provide 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 *Uncertainties*—The inherent sampling uncertainty of the Monte Carlo method can be estimated as a Type A 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 run. In addition, there are Type B 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 Type B uncertainties can be estimated by analytical techniques. Various elements of the calculation can be validated with dosimetry.

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 **(24-28)**. 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 **(29)**. All of these methods place limits on the angular variable such that the particles are 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 2D and 3D has been done by several workers **(30-35)**.

5.4.2 *Point Kernel Methods*—Point kernel methods are used mainly for photon transport problems **(36)**. In point kernel methods, the radiation source volume is approximated by a number of isotropic point sources. The total 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 3—There are a number of general databases available for the gamma-ray buildup factors needed for these codes (Annex A1). See also section 7.1.4 of reference **(36)** on the point kernel applications of buildup factors.

5.4.3 *Advantages*—Deterministic methods are typically faster than Monte Carlo, and can be benchmarked against dosimetry. For single dose points, the Monte Carlo method is faster. For multiple dose points, discrete ordinates methods are faster.

5.4.4 *Disadvantages*—Deterministic methods give no innate estimate of precision. 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 (see for example, reference **(37)**).

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). Dose interpolation is based on facility and product-specific characteristics. The model equations are typically specific to a particular 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 **(38)**, electron energy loss **(39)** and depth-dose relationships in various materials **(40)**.

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 provides 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 **(41-47)**.

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 and/or irradiation applications 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 4—If a one-dimensional model such as the semi-empirical EDMULT code (A1.2, **(43)**) is used to obtain an estimate of the dose in a system that is finite in more than one dimension, checking the dose with a 2-D or 3-D Monte Carlo simulation is recommended.

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 dosimetry.

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.

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 5—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, photons 200 keV and above in energy Compton scatter from cell/source walls and make a large and broad low energy contribution to the spectrum.

6.2 *Personnel*—Experienced 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 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.

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 resolution are important. If the problem must be further broken down into smaller regions of different material (density) in order to achieve accuracy, more complex input files will be needed. 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 long run times, 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) **(37,48,49)**.

7.2.3 *Precision and Accuracy*—The Monte Carlo method is the only method that generates an estimate of precision (in the sense of convergence of solutions) as part of the calculation. While precision and accuracy are terms generally used with respect to sampling, the accuracy of any method will depend on the detail that has been included in the model. See Terminology E 170 and Practice 51707.

7.2.4 *Set-up Time*—The complication 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 model set-up, execution and evaluation-related times 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 sought, 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 and/or Monte Carlo solutions may be sought.

NOTE 6—Deterministic and/or stochastic approaches may be utilized for the expressed purpose of supplementing a sparse measurement database so that empirical relationships can be established and employed.

NOTE 7—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 and/or Monte Carlo solutions. 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 shall be done using a comprehensive measurement database (dosimetry results). See Section 8 concerning validation.

8. Verification and Validation of Model Performance

8.1 *Verification and Validation*—Validation compares the code output to results of an appropriate experiment. Verification demonstrates that theory was implemented in a mathematically correct manner, and that the simulation was built in accordance with its requirements and specifications. Both verification and validation of a model require the use of a comprehensive measurement database of dosimetry results and other accepted calculations. Although these are important concepts, in practice verification and validation are often co-mingled 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 A4. An example comparing the results of several methods (Monte Carlo, deterministic and semi-empirical) with dosimetry can be found in reference **(50)**.

NOTE 8—One form of verification exercise that is common in the area of computer-based modeling is benchmarking. 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).

8.2 *Validation*—Formal software testing is not addressed in this guide. When available or feasible, 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 have GMP or ISO implications. Refer to Annex A2 for references and Guide E 482 for further guidance on software validation.

NOTE 9—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.

8.3 *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.

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

8.4.1 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.

9. Uncertainty in Model/Method Prediction

9.1 The calculation of absorbed dose should be compared with the measurement of absorbed dose. The required degree of agreement between calculation and measurement depends on the user's requirements.

9.1.1 Refer to 2.1 for ASTM standards on dosimetry methods and uncertainties.

9.1.2 A detailed uncertainty analysis (Type A and B) for the calibration and use of thin film dosimeters and PMMA can be found in references **(51,52)**.

9.2 The Monte Carlo method does provide an estimate of precision only insofar as it relates to the calculation. Biasing due to variation in geometry and composition of the irradiated products, and in the properties of the source are additional sources of systematic uncertainty; see Terminology E 170 and Practice 51707.

9.3 The verification and validation procedure should be documented and rigorously adhered to by both the modeler and the experimenter. Inadequate description of the problem and coding errors constitute a significant source of uncertainty. Inherently, all models are approximations and limitations to geometry description and approximations to the actual physics will cause calculated values to differ from standards. 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. While gross errors are easily caught, subtle errors in algorithms contribute to the overall uncertainty.

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.

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 cutoffs, 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 10—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 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 cutoff).

10.3.3 Sufficient information 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*:

10.4.1 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*:

10.6.1 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.

10.6.2 References to all files associated with verification and/or validation of modeling software performance.

11. Keywords

11.1 benchmarking; deterministic method; discrete ordinates; empirical method; mathematical models; modeling; modelling; Monte Carlo method; 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 and PENELOPE are available from RSICC (Radiation Safety Information Computational Center), Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831-6362, USA. See A1.10 for source of ITS and other codes in Europe.

A1.2 The Monte Carlo code MCBEND is available from AEA Technology plc, Winfrith, Dorchester, Dorset DT2 8DH United Kingdom.

A1.3 The adjoint Monte Carlo code NOVICE is available from EMPC, PO Box 3191, Gaithersburg, MD 20885, USA.

A1.4 The point kernel code QAD-CGGP is available from RSICC.

A1.5 The point kernel code RANKERN is available from AEA Technology plc, Winfrith, Dorchester, Dorset DT2 8DH United Kingdom.

A1.6 The point kernel code PK-MASTER is available from Special Process Services L.C., Box 605, Dunn Loring, VA 22027, USA.

A1.7 The coupled electon/photon discrete ordinates code CEPXS/ONELD and photon codes DANTSYS and TORT are available from RSICC.

A1.8 The semi-empirical code EDMULT is available from RSICC.

A1.9 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. The newsletter is available from Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831-6362, USA. Phone 865-574-6176, FAX 865-574-6182; Web Address: PDC@ORNL.GOV; WWW: http://www-rsicc.ornl.gov/rsic.html.

A1.10 Information related to computer codes and data banks, GEANT Library, nuclear safety, radiation protection, publications and press releases can be accessed from the OECD Nuclear Energy Agency, Le Seine Saint-Germain, 12 boulevard des Iles, 92130 Issy-les-Moulineaux, FRANCE. Tel: +33 (0) 1 4524 8200, Fax: +33 (0) 1 4524 1110; Web Address: www.nea.fr.

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

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.

A2.2 FDA Medical Device Quality System Manual, Design Control Guidance For Medical Device Manufacturers, March 1997, 2098 Gaither Road, Rockville, Maryland 20850, USA.

A2.3 Guidelines for the Application of ANSI/ISO/ASQC 9000-3-1991 to the Development, Supply, & Maintenance of Software, American Society for Quality (Control) ASQ, P.O. Box 3005, Milwaukee, WI 53201- 3005, USA.

A2.4 Software Quality Assurance—A Guide For Developers and Auditors, Howard T. Garston Smith, Interpharm Press, Inc., 1358 Busch Parkway, Buffalo Grove, IL 60089, USA, ISBN: 1-57491-049-3-1997.

A2.5 Validation Compliance Annual—1995, International Validation Forum, Inc., Marcel Dekker, Inc., 270 Madison Ave., New York, NY 10016, USA, ISBN: 0-8247-9459-1-1995.

A2.6 Computer Systems Validation for the Pharmaceutical and Medical Device Industries, Richard Chamberlain, Alaren Press, 1117 S. Milwaukee Ave., Suite B, Libertyville, IL 60048, USA, ISBN: 0-9631489-0-8-1994.

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

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

A2.9 Saylor, M. C., Baryschpolec, S. W., Hurwitz, L. M., and McLaughlin, W. L., "Radiation Process Data Collection, Analysis, and Interpretation," in *Sterilization of Medical Products*, Volume VI, Morrisey, R. F., ed., Polyscience Publications Inc., Morin Heights, Quebec, Canada; pp. 240-260, 1993.

A3. PHYSICS AND MODELING TUTORIAL

Several useful and well-known textbooks are available on the subjects of shielding **(36)** and transport methods **(53,54)**.

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, where dose uniformity is not as good as with gamma rays, alternative product packaging designs may be considered to optimize dose uniformity, throughput and 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. It is never possible or practical to create an exact model of reality; therefore 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 experienced 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 **(55,56)**. Absorbed dose is a measure of the energy deposited per unit mass (refer to ICRU references for definitions and unit equivalents). 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. High-energy 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-rays and bremsstrahlung) deposit energy over greater distances than electrons. They are also the primary reason that radiation shielding is necessary. Electrons, on the other hand, have charge and mass. Therefore, accelerated electrons have a high number of interactions per unit path

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.

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 beams are capable of sending electrons 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. This causes sharp changes in dose (sometimes known as the "dose enhancement effect") at interfaces where materials of different densities and/or atomic number meet (see **(57)** and references contained therein). 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 generally be assumed to be inadequate. Attending a course or workshop for a particular code is recommended for the less-experienced user. 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. 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 truly three-dimensional method capable of including all of the radiation transport physics and, therefore, all the scattering effects necessary to get accuracy. These codes are very sophisticated and actually mimic the real world. The model is sampled to provide a prediction with an indication of precision. A sample is a batch of particle histories that is only a small fraction of the real population of particles experienced in the real world. The dose calculation based on a single small sample will contain a large and unknown amount of imprecision. However, as the size of the sampling increases, the method converges on a result 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 (e.g. 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. ANNOTATED EXAMPLES

A4.1 *Examples for Monte Carlo Models:*

A4.1.1 Several general articles on Monte Carlo techniques and applications are cited in the references **(5,18,58-60)** including the original article on condensed history Monte Carlo **(61)**.

A4.1.2 A comparisons 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 reference **(54)**.

A4.1.3 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 reference **(54)**. A strategy for determining dose-depth relationships in standard construction geometries for a wide variety of applications using ITS can be found in reference **(62)**.

A4.1.4 A comparison between the simple-geometry examples for the EGS code system can be found under "Experimental Benchmarks of EGS," and "Positron Emission Tomography Applications of EGS" in reference **(54)**.

A4.1.5 A sensitivity study for including/omitting the titanium beam window and air gap for 400 keV electrons impinging on a nylon substrate can be found in Fig. 6 of reference **(56)**.

A4.1.6 An example of verification of a Monte Carlo code for thick target bremsstrahlung calculations can be found in reference **(63)**.

A4.1.7 Comparisons between Monte Carlo codes with regard to dosimetry at material interfaces, backscatter factors and depth-dose curves can be found in references **(64,65)**.

A4.1.8 A comparison of pencil beam algorithms with Monte Carlo methods can be found in reference **(66)**.

A4.1.9 Simulations of a variety of detectors/scintillators (thermoluminescent, silicon, sodium iodide, lithium fluoride, and diamond) can be found in references **(67-72)**.

A4.1.10 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 references **(73-75)**. 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 reference **(76)**.

A4.1.11 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 reference **(77)**. The same approach was later applied to other moving objects (bottles) in reference **(78)**. 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 reference **(79)**.

A4.1.12 Several Monte Carlo gamma irradiation processing facility validation studies, including process planning and dose rate determinations, using MCNP can be found in **(80-83)**. 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.

A4.1.13 An application of EGS4 for determination of gamma ray spectrum and dose rate distribution in a Gamma-Cell 220 can be found in **(84)**.

A4.2 *Examples of Deterministic Models:*

A4.2.1 *Annotated Examples for the Discrete Ordinates Method*:

A4.2.1.1 Simple one-dimensional geometry comparisons to experiment and Monte Carlo methods can be found in **(20)**.

A4.2.1.2 Simple geometry one-dimensional and two-dimensional comparisons can be found in reference **(85)**.

A4.2.1.3 Forward and adjoint methods and applications can be found in reference **(26)**.

A4.2.1.4 Efficient modeling of Compton diode gamma-radiation detectors can be found in reference **(86)**.

A4.2.1.5 A comprehensive comparison of CEPXS/ONELD calculations with the ^{60}Co data set of Wall and Burke can be found in reference **(57)**.

A4.2.1.6 A comparison of ONETRAN calculations with dosimetry measurements for electron beam dose profiles can be found in reference **(87)**.

A4.2.1.7 A comparison of ONETRAN calculations with dosimetry measurement for ^{60}Co dose profile data to determine photon spectrum can be found in reference **(88)**.

A4.2.2 *Annotated Examples for the Point Kernel Method*:

A4.2.2.1 Annotated examples for the point kernel method can be found in reference **(36)**.

A4.2.2.2 A study of gamma ray buildup factors for a point isotropic source in stratified shields can be found in reference **(49)**.

A4.2.2.3 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 **(6,89)**. Detailed model descriptions of actual product (Petri dishes) provided good agreement (3 to 8 %) with dosimetry using QAD-CGGP code **(90)**. For routine screening, a less precise (15 % uncertainty) but simpler and faster code was a better approach **(91)**.

A4.2.2.4 Dose distribution predictions for a range of product densities have been mapped at high resolution (60 cm^3) to assess sterility assurance **(92)**.

A4.2.2.5 Advanced examples of application of point kernel codes to industrial radiation processing **(48)**, process control charting **(93)**, "off-carrier" processing **(94)** and source rack loading planning **(95)** have recently appeared.

A4.3 *Examples of Empirical and Semi-empirical Models:*

A4.3.1 *Annotated Examples for the Empirical Method*:

A4.3.1.1 Empirical expressions for beta-ray point-source dose distributions can be found in reference **(96)**.

A4.3.1.2 Analytical fits of empirical equations to Monte Carlo calculated depth dose curves for 1 to 50 MeV electrons in water can be found in reference **(97)**.

A4.3.2 *Annotated Examples for the Semi-empirical Method*:

A4.3.2.1 An algorithm for depth-dose curves of electrons fitted to Monte Carlo data can be found in reference **(98)**.

A4.3.2.2 A discussion of the EDMULT code can be found in reference **(99)**.

A4.3.2.3 A comparison of calculated and measured absorbed doses of electron beams can be found in reference **(100)**.

A4.3.2.4 Extension of EDMULT code for calculation of dose distribution in tubing and comparison with dosimetry can be found in reference **(101)**.

A5. PARTICULARS OF THREE-DIMENSIONAL MODEL CONSTRUCTION

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

A5.1 *General*—The model should contain all elements that will affect absorbed dose and dose distribution of the geometry in question. 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.

A5.1.1 The source of the radiation should be accurately described and include its dimensions and energy. The geometry details of the irradiator should be accurately described using direct measurements or verification of physical drawings where applicable.

A5.1.2 Some simplification of elements may be necessary (cobalt linear sources, steel rollers) in order to reduce the number of input bodies. Care must be exercised to maintain mass and dimensions.

A5.1.3 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.

A5.1.4 The need to tailor the model for the specific application may involve code modification, modifications to the geometry to factor 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 (e.g. a user interface).

A5.1.5 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.

A5.2 *Photon Source Model Construction:*

A5.2.1 For a photon source the model could typically include such things as linear arrays of isotope and metal structural components that interact with the radiation environment sufficiently to affect the absorbed dose distribution in the product.

A5.2.2 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.

A5.3 *Electron Source Model Construction:*

A5.3.1 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. Use of scatter plates to redirect "escaping" electrons back towards the product may also be a consideration.

A5.3.2 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.

A5.4 *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.

A5.4.1 *Electron Beam*—Small or focused sources (electron beam) can be modeled as distributed sources to factor into the dose calculation the movement of the product through the radiation field with time **(77,78)**.

A5.4.2 *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.

A5.5 *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.

A5.6 *Model of a Facility Using Specific Products:*

A5.6.1 For the product, the geometry would include detailed descriptions of the bodies broken down into components of density, composition and dimensions.

A5.6.2 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.

A5.6.3 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.

A5.7 *Model of Dosimeters:*

A5.7.1 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.

A5.7.2 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.

A5.7.3 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. 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 type of error.

A5.7.4 Dose predictions must be validated by irradiating actual product with dosimeters in specific locations.

A5.8 *Dose Calculation:*

A5.8.1 For an electron beam model where the dose calculation is expressed as energy deposited (MeV) per source electron (E) per gram (g), conversion to units of kilograys may be achieved using the lump sum conversion factor of 1000 kilogray·cm^2/mA·s multiplied by the actual beam operating parameters (I = beam current in mA and A (cm^2) = area irradiated). The lump sum conversion factor is derived from the following equivalents:

$$1 \text{ kilogray} = 6.24 \times 10^{12} \text{ MeV/g}$$

and

$$1\text{mA} = 6.24 \times 10^{15} \text{ electrons·cm}^2\text{/s}$$

and

$$1 \text{ MeV·cm}^2\text{/g·electron} =$$

$$[1.6 \times 10^{-13} \text{ kGy·cm}^2\text{/electron}]\,[1 \text{ electron}/1.6 \times 10^{-16} \text{ mA·s}]$$
$$= 1000 \text{ kGy·cm}^2\text{/mA·s}$$

Absorbed Dose (D) Conversion for an Electron Beam:

$$D \text{ (kGy (material))} = \frac{1000\, E \text{ (MeV)}\, I \text{ (mA)}}{\text{g}\, A \text{ (cm}^2\text{)}}$$

A5.8.1.1 Suitable modifications to this simple equation may be required to adjust the calculation for movement of product through the radiation field.

A5.8.2 For a gamma ray model where the dose calculation is expressed as energy deposited (MeV) per photon (E) per gram (g), conversion to units of kilograys may be achieved using the lump sum conversion factor of 5930 kilogray·cm^2/MCi·s multiplied by the actual operating parameters (S = source strength in MCi and t = residence time in seconds). The lump sum conversion factor is derived from the following equivalents; 1 kilogray = 6.24×10^{12} MeV/g and 1 megacurie (MCi) = 3.7×10^{16} disintegrations/s. The unit cancellations are shown below.

$$\text{Absorbed Dose (kGy)} =$$

$$\frac{\text{E [MeV/}\gamma\text{]}\; S \text{ [MCi]}\; [3.7 \times 10^{16}\; \gamma\text{/s/MCi}]\; t \text{ [s]}\; [1 \text{ kGy/ } 6.24 \times 10^{12} \text{ MeV/g}]}{\text{Vol [cm}^3\text{]}\; \rho \text{ [g/cm}^3\text{]}}$$

Absorbed Dose Conversion (D) for a Gamma Source:

$$D \text{ (kGy (material))} = \frac{5930\, E \text{ (MeV)}\, S \text{ (MCi)}\, t \text{ (s)}}{\text{g}}$$

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