



Standard Guide for Selection and Use of Mathematical Methods for Calculating Absorbed Dose in Radiation Processing Applications¹

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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 ¹³⁷Cs or ⁶⁰Co, 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**.

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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 Dosimetry²

E482 Guide for Application of Neutron Transport Methods for Reactor Vessel Surveillance, E706 (IID)²

E666 Practice for Calculating Absorbed Dose From Gamma or X Radiation

2.2 ISO/ASTM Standards:

51204 Practice for Dosimetry in Gamma Irradiation Facilities for Food Processing²

51275 Practice for Use of a Radiochromic Film Dosimetry System²

51400 Practice for Characterization and Performance of a High-Dose Radiation Dosimetry Calibration Laboratory²

51431 Practice for Dosimetry in Electron and Bremsstrahlung Irradiation Facilities for Food Processing²

51608 Practice for Dosimetry in an X-ray (Bremsstrahlung) Facility for Radiation Processing²

51649 Practice for Dosimetry in an Electron Beam Facility for Radiation Processing at Energies between 300 keV and 25 MeV²

51702 Practice for Dosimetry in a Gamma Irradiation Facility for Radiation Processing²

51707 Guide for Estimating Uncertainties in Dosimetry for Radiation Processing²

51818 Practice for Dosimetry in an Electron Beam Facility for Radiation Processing at Energies between 80 and 300 keV²

51939 Practice for Blood Irradiation Dosimetry²

2.3 International Commission on Radiation Units and Measurements Reports:³

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

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

3.1.4 *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*.

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.

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 E170. Definitions in Terminology E170 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 in-nate 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, ⁶⁰Co 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 E170 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.