~~Designation:E2232–02~~ Designation: E2232 – 10

An American National Standard

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

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

1. Scope

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

1.2 Radiation processing is an evolving field and annotated examples are provided in Annex ~~A4~~A6 to illustrate the applications where mathematical methods have been successfully applied. While not limited by the applications cited in these examples, applications specific to neutron transport, radiation therapy and shielding design are not addressed in this document.

1.3 This guide covers the calculation of radiation transport of electrons and photons ~~in the energy range of 0.1~~with energies up to 25 MeV.

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

1.5 General purpose software packages are available for the calculation of the transport of charged and/or ~~neutral~~uncharged 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.~~

~~1.6This 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.~~ Co, for energetic electrons from particle accelerators, or for X-rays generated by electron accelerators.

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

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

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

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E170 Terminology Relating to Radiation Measurements and Dosimetry

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

~~E666Practice for Calculating Absorbed Dose From Gamma or X Radiation~~ Guide for Application of Neutron Transport Methods for Reactor Vessel Surveillance, E706 (IID)

2.2 ~~*ISO/ASTM Standards:*~~

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

[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 Radiation Processing: Dosimetry and Applications.

~~Current edition approved Sept. 10, 2002. Published November 2002. DOI: 10.1520/E2232-02.~~

Current edition approved July 1, 2010. Published September 2010. Originally approved in 2002. Last previous edition approved in 2002 as E2232-02. DOI: 10.1520/E2232-10.

[2] For referenced ASTM and ISO/ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* ~~, Vol 12.02.~~volume information, refer to the standard's Document Summary page on the ASTM website.

51275Practice for Use of a Radiochromic Film Dosimetry System[2]
51400Practice for Characterization and Performance of a High-Dose Radiation Dosimetry Calibration Laboratory[2]
51431Practice for Dosimetry in Electron and Bremsstrahlung Irradiation Facilities for Food Processing[2]
51608Practice for Dosimetry in an X-ray (Bremsstrahlung) Facility for Radiation Processing[2]
51649Practice for Dosimetry in an Electron Beam Facility for Radiation Processing at Energies between 300 keV and 25 MeV[2]
51702Practice for Dosimetry in a Gamma Irradiation Facility for Radiation Processing[2]
ISO/ASTM Standards:[2]
51707Guide for Estimating Uncertainties in Dosimetry for Radiation Processing[2]
51818Practice for Dosimetry in an Electron Beam Facility for Radiation Processing at Energies between 80 and 300 keV[2]
51939Practice for Blood Irradiation Dosimetry[2]
2.3 *Guide for Estimating Uncertainties in Dosimetry for Radiation Processing*
2.3 *International Commission on Radiation Units and Measurements Reports:*[3]
ICRU Report 14,Radiation Dosimetry: X-Rays and Gamma 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:*
ICRU Report 60 Fundamental Quantities and Units for Ionizing Radiation
ICRU Report 80 Dosimetry Systems for Use in Radiation Processing
2.4 *United States National Institute of Standards and Technology:*[4]
ISO 9001Quality Systems—Model for Quality Assurance in Design/Development, Production, Installation and Servicing
ISO 9002Quality Systems—Model for Quality Assurance in Production and Installation
ISO 11137Sterilization of Health Care Products—Requirements for Validation and Routine Control - Radiation Sterilization
NIST Technical Note 1297 (1994 edition) Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results

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

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

3.1.2 *biasing—in (in a Monte Carlo simulation, an adjustmentsimulation)*—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.

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

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

[3] Available from International Commission on Radiation Units and Measurements, 7910 Woodmont Ave., Suite 800, Bethesda, MD 2081420815 USA.
[4] Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036 USA.
[4] Available as a download from the NIST web site at: http://physics.nist.gov/Pubs/guidelines/TN1297/tn1297s.pdf.

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~~method*—a method derived from fitting an approximating function to experimental data or Monte Carlo calculation ~~result.~~ 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~~history*—a particle history is the record of all simulated interactions along its track as used in stochastic ~~or Monte Carlo simulations.~~ simulations (for example, Monte Carlo).

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

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

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

3.1.11 *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.~~ radiation with matter.

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

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

physical processes in the system being studied. A random variable is a variable whose value is a function of a statistical distribution of random values.

3.1.17.1 *Discussion*—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 integro-differential equation describing the motion of particles or radiation through a medium. ~~This~~

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

3.1.19 ~~*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.~~ Type A evaluation (of standard uncertainty)—method of evaluation of a standard uncertainty by the statistical analysis of a series of observations.

3.1.19.1 *Discussion*—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.

3.1.20 *Type B evaluation (of standard uncertainty)*—method of evaluation of a standard uncertainty by means other than the statistical analysis of a series of observations.

3.1.20.1 *Discussion*—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. A Type B uncertainty could result from the difference in geometry and material composition of the modelled irradiator versus the actual irradiator. Other sources of Type B uncertainty are the inadequate description of the problem and approximations to actual physics.

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

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

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

~~3.1.20.1~~

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

~~3.1.21~~

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

~~3.1.21.1~~

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

~~3.1.22~~3.1.24 *zoning*—The geometric description used to break up a larger region into smaller segments in which to calculate the dose.

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

3.2 Definitions of other terms used in this standard that pertain to radiation measurement and dosimetry may be found in Terminology E170. Definitions in Terminology E170 are compatible with ICRU ~~51~~60 and ~~60~~80; 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 the 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.~~ —Verification is the confirmation of the mathematical correctness of a computer implementation of a mathematical method. This can be done, for example, by comparing numerical results with known analytic solutions or with other computer codes that have been previously verified. Verification should be done to ensure that the simulation is appropriate for the intended application. Refer to 3.1.23.1.

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

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

4.10 This guide should not be used as the only reference in the selection and use of mathematical models. The user is encouraged to contact individuals who are experienced in mathematical modelling and to read the relevant publications in order to select the best tool for their application. Radiation processing is an evolving field and the references cited in the annotated examples of Annex ~~A4~~A6 are representative of the various published applications. Where a method is validated with dosimetry, it becomes a benchmark for that particular application.

5. Classification of Mathematical Methods and General Application

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

5.2 *Types of Methods*—Four general types of ~~models~~methods are in use: Monte Carlo, deterministic, semi-empirical and empirical. Both Monte Carlo and deterministic ~~models~~methods 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~~ a finite number of photons or electrons~~)~~ and estimating dose by summing and averaging the histories of many ~~particles.~~ energy deposition events.

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

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

5.3 *Monte Carlo Method*—The Monte Carlo method simulates the paths of particles such as electrons and photons from the source to the ~~target.~~dose volume. See Note 1~~, references~~ **, Refs (10-23) and Annex A1 ~~for examples and codes.~~ for examples and codes. See also A3.3 and A3.4.4 for brief discussions of the physics of electron and photon transport and the Monte Carlo method respectively.**

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

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~~ —Because electrons (including those generated by photons) in the energy range of 50 keV to 10 MeV undergo large numbers of scattering events, exact simulation of all photon and electron paths is not feasible or practical. Instead, approximate electron paths are employed, as in the so-called "condensed history Monte Carlo method" **(24-27)**. For electrons, approximate artificial trajectories using large path length steps and a multiple-scattering approach to particle deflections are employed in standard Monte Carlo codes. (See Annex A1~~). Such approximate paths may lead to significant errors, particularly when transport across surfaces or material interfaces is important.~~ .) The standard Monte Carlo codes listed in Annex A1 and references **(10-23)** use this condensed history approach. However, such approximate paths may lead to significant errors,

particularly at locations where transport across surfaces or material interfaces is important. See Note 4.

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

NOTE 4—In some Monte Carlo codes (**21**), improved accuracy near material boundaries has been obtained using shorter paths near interfaces between different materials.

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

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

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

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

5.3.3 ~~*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.~~ Type A Uncertainty—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 histories. For calculations without biasing, the statistical uncertainty scales as the reciprocal of the square root of the number of histories run.

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

5.3.4 *Type B Uncertainty*—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.

NOTE 6—There is great potential for large discrepancies in results because there is no estimate of Type B uncertainty from software. Refer to Section 9.

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**~~(**28-32**). 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**~~(**33**). All of these methods place limits on the angular variable such that the ~~particles are~~ incident radiation is represented as streaming only along a finite number of directions rather than all possible directions as contained in the transport equation. Extension of this technique to 2-D and 3-D has been done by several workers (~~**30-35**~~**34-39**).

5.4.2 *Point Kernel Methods*—Point kernel methods are used mainly for photon transport problems ~~(**36**~~(**40**). 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~~ 7—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.~~ —Deterministic methods may be faster than Monte Carlo, and can be benchmarked against dosimetry.

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

5.4.5 *Uncertainties*—There are three sources of uncertainties in deterministic models. These are ~~(1)~~*(1)* the approximations used to create physical models and cross-sections (for example, energy straggling is neglected in deterministic methods), ~~(2)~~ *(2)* the effect of representing a continuous problem in space, angle and energy with a finite mesh in all these variables and ~~(3)~~*(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~~**41**~~))~~. .

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**~~**42**~~**)**, electron energy loss ~~**(39**~~**(43)** and depth-dose relationships in various materials ~~**(40**~~**(44)** .

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~~provide a more generally applicable mathematical model than the empirical method and are adjustable to physical parameters of the facility, source and products, such as energy, density and composition. In general, these are software-based programs with variable parameter inputs. Equations, codes and databases are available (~~**41-47**~~**45-51**).

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~~ 8—If a one-dimensional model such as the semi-empirical EDMULT code (~~A1.2~~A1.9, ~~(43~~**(47)**) is used to obtain an estimate of the dose in a system that is finite in more than one dimension **(52)**, 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*:

~~6.1.1Detailed drawings of irradiation facility equipment, source-related equipment and associated geometries, should be obtained, physically verified, and documented.~~

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

NOTE 9—Fig. 1 shows a solid model of a typical gamma irradiator with product in aluminum totes. For clarity, four totes and part of the source shroud have been removed. The tote irradiator uses a shuffle-and-dwell concept. Each product tote is irradiated for a defined period of time before each tote is indexed to the next irradiation positions. The source rack containing the radiation sources is shown **(53)**.

NOTE 10—Fig. 2 shows a photograph of research carrier and the graphical user interface window of a mathematical model. All product is contained aluminum totes. For the research carrier, product is brought into the irradiator and irradiated for a defined period of time, and then leaves the irradiation chamber. The graphical user interface shows ray tracing between the radiation source and the dose volume **(53)**.

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~~ 11—In the case of gamma-ray sources (for example, ^{60}Co sources), the photon energy spectrum may be difficult to obtain experimentally or estimate theoretically. In general, for photons with energies 200 keV and ~~above in energy Compton scatter from cell/source walls and make~~ above,

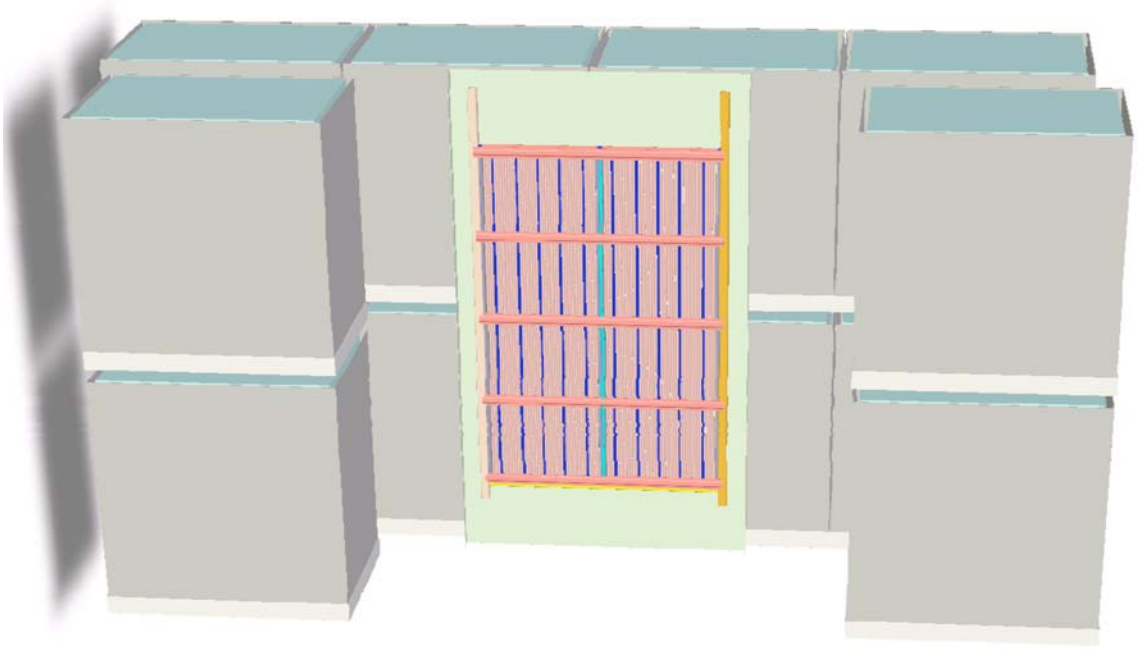

FIG. 1 Solid Model of a Gamma Production Irradiator (53)

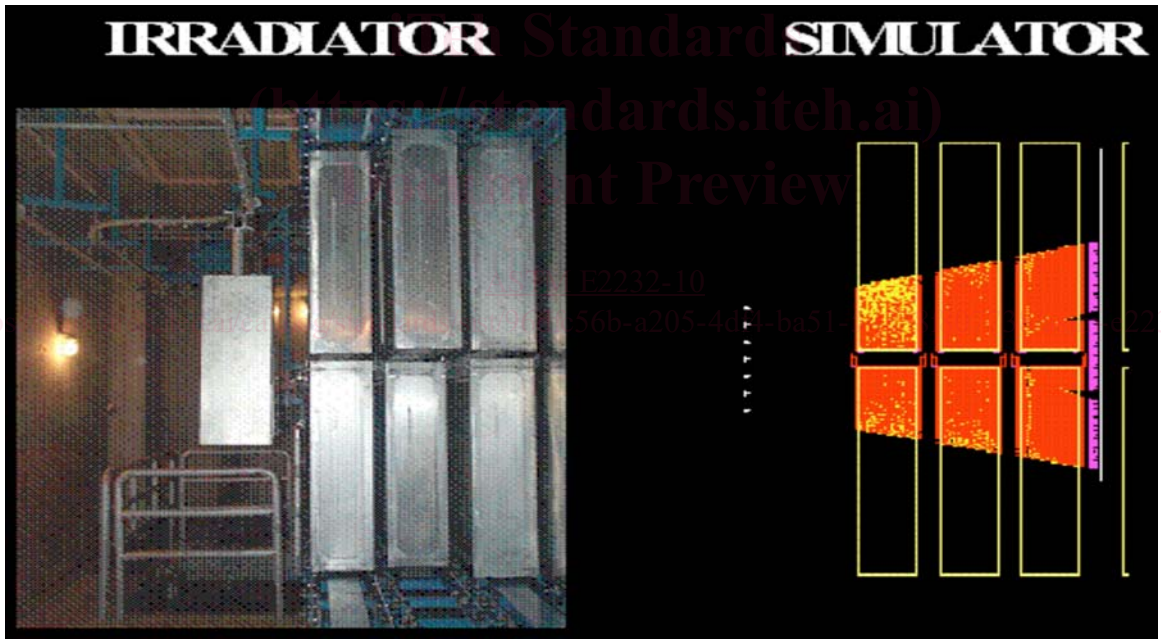

FIG. 2 Picture and Simulation of a Gamma Production Irradiator and Research Loop (53)

a ~~large and~~ broad low energy contribution to the spectrum is created via Compton scattering.

6.2 *Personnel*—~~Experienced~~—Trained personnel should be involved in all aspects of model development, program execution, data reduction and the evaluation of results. There is no standard set of qualifications that can be recommended. Interaction of personnel with all phases of the modeling exercise should be documented according to the end-user's policy and procedural 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~~ (see also 7.2~~.~~ ~~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.

7.2.2.1 Available software may have geometry replication and tiling features that are very useful for this purpose. If the target size is small relative to geometry or source description, Monte Carlo may require ~~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~~41,~~48~~54,~~49~~55)**.

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,~~developed, evaluated against experimental results and, when found to satisfy written criteria within the limits established in the documentation, accepted and applied.

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

NOTE ~~6~~12—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~~13—Because of the more rigorous physical models used in Monte Carlo codes, these may be considered for the purpose of verifying or validating performance of a proposed deterministic or empirical solution.

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

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

8. Verification and Validation of Model Performance

8.1 *Model Verification and Validation*—Validation compares the code output to results of an appropriate experiment.

Verification ~~demonstrates~~confirms that the theory was implemented in a mathematically correct ~~manner, and that the simulation was built in accordance with its requirements and specifications.~~ manner. 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~~efforts often ~~co-mingled~~overlap during model testing.

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

8.1.1.1 There are a limited number of referenced benchmark examples in the literature and these may be inadequate in number to validate a method and inadequate in detail for comparison with the model under consideration. The model of the application of interest should be as nearly the same as possible to the benchmark example. Benchmark examples may be found in Annex ~~A4~~A5. An example comparing the results of several methods (Monte Carlo, deterministic and semi-empirical) with dosimetry can be found in ~~reference~~Ref **(~~50~~56)**.

~~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 E482 for further guidance on software validation.~~ 14—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).

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

~~8.3~~

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

~~8.4~~

8.3 *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.**~~

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

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

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

9. Uncertainty in Model/Method Prediction

~~9.1 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 Similar to dosimetric measurement, an estimate of uncertainty accompanies dose calculations. As a minimum, an estimate of the calculation accuracy can be ascertained by taking the ratio of the calculation of absorbed dose and the measurement of absorbed dose (when the measurement is traceable to a national standard). The accepted degree of agreement between calculation