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

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

1. Scope

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

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

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

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

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

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

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

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

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E170 Terminology Relating to Radiation Measurements and Dosimetry

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

2.2 *ISO/ASTM Standards:*[2]

51707 Guide for Estimating Uncertainties in Dosimetry for Radiation Processing

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

ICRU Report ~~60~~85a Fundamental Quantities and Units for Ionizing Radiation

~~ICRU Report 80 Dosimetry Systems for Use in Radiation Processing~~

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

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

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

2.4 *United States National Institute of Standards and Technology:*[4]
NIST Technical Note 1297 (1994 edition) Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results

3. Terminology

3.1 *Definitions:*

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

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

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

3.1.2.1 *Discussion*—

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

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

3.1.3.1 *Discussion*—

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

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

3.1.4.1 *Discussion*—

The concept of build-up applies to the transport of photons.

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

3.1.5.1 *Discussion*—

The point kernel and discrete ordinate methods are examples of deterministic methods.

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

3.1.6.1 *Discussion*—

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

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

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

3.1.7.1 *Discussion—*

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

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

3.1.8.1 *Discussion—*

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

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

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

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

3.1.11.1 *Discussion—*

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

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

3.1.12.1 *Discussion—*

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

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

3.1.13.1 *Discussion—*

The point kernel method is typically used for photon transport applications. The radiation source is modeled as a large set of point sources. The absorbed dose, dose equivalent or exposure is estimated at a dose point by integrating the contribution from each of the point sources. A multiplicative value (the semi-empirical build-up factor) is used to account for the contribution from scattered (indirect) radiation from regions not in the direct path between the source point and field point.

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

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

3.1.15.1 *Discussion—*

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

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

3.1.16.1 *Discussion*—

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

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

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

3.1.18.1 *Discussion*—

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

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

3.1.19.1 *Discussion*—

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

~~3.1.18 *transport equation*—an integro-differential equation describing the motion of particles or radiation through a medium.~~

~~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 *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)*—~~*non-statistical component of uncertainty*—~~method of evaluation of a standard uncertainty~~ component of uncertainty evaluated by means other than ~~the~~ statistical analysis of a series of ~~observations.~~calculated values.

3.1.20.1 *Discussion*—

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

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

3.1.21.1 *Discussion*—

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

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

3.1.22.1 *Discussion*—

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

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

3.1.23.1 *Discussion*—

Validation compares a code or theory with results of an appropriate experiment.

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

3.1.24.1 *Discussion*—

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

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

3.1.25.1 *Discussion*—

Partitioning a zone into smaller segments is referred to as subzoning.

3.2 Definitions of other terms used in this standard that pertain to radiation measurement and dosimetry may be found in Terminology E170. Definitions in Terminology E170 are compatible with ICRU ~~60 and 80;~~ 85a; those documents, therefore, may be used as alternative references.

4. Significance and Use

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

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

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

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

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

4.6 *Facility Design*—Dose calculations are often used in the design of a new irradiator and can be used to help optimize dose distribution in an existing facility or radiation process. The use of modeling in irradiator design can be found in ~~references~~Refs (**~~3~~-2-~~79~~**).

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

4.8 *Verification*—Verification is the confirmation of the mathematical correctness of a computer implementation of a mathematical method. This can be done, for example, by comparing numerical results with known analytic solutions or with other

computer codes that have been previously verified. Verification should be done to ensure that the simulation is appropriate for the intended application. Refer to 3.1.24~~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 ~~determination~~measurement (refer to ISO/ASTM 51707 and NIST Technical Note 1297). In many cases, absorbed-dose measurement helps to establish the uncertainty in the dose calculation.

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

5. Classification of Mathematical Methods and General Application

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

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

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

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

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

5.3 *Monte Carlo Method*—The Monte Carlo method simulates the paths of particles such as electrons and photons from the source to the dose volume. See Note 1, Refs (~~10-8-1923~~) and Annex A1 for examples and codes. See also A3.3 and A3.4.4 for brief discussions of the physics of electron and photon transport and the Monte Carlo method respectively.

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

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

5.3.2 *Disadvantages*—Because electrons (including those generated by photons) in the energy range of 50 keV to 10 MeV undergo large numbers of scattering events, exact simulation of all photon and electron paths is not feasible or practical. Instead, approximate electron paths are employed, as in the so-called "condensed history Monte Carlo method" (~~24-~~20 and 21~~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.) The standard Monte Carlo codes listed in Annex A1 and ~~references~~Refs (~~10-8-1923~~) 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 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~~17), improved accuracy near material boundaries has been obtained using shorter paths near interfaces between different materials.

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

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

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

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

5.3.3 *~~Type A~~ Statistical Uncertainty*—The inherent ~~sampling uncertainty of~~ uncertainty in the calculated value of dose due to sampling in 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~~ Non-statistical Component of 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.~~ These uncertainties can be estimated by analytical techniques, which may include sensitivity analysis (changing a value of a parameter by an amount related to its uncertainty and rerunning the calculation to compare the results. Various elements of the calculation can be validated with dosimetry.

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

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

5.4.1 *Discrete Ordinates Methods*—These methods have been used for both electron and photon sources (**~~28~~-22 and 2332**). 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 (**3324**). All of these methods place limits on the angular variable such that the incident radiation is represented as streaming only along a finite number of directions rather than all possible directions as contained in the transport equation. Extension of this technique to 2-D and 3-D has been done by several ~~workers~~authors (**~~34~~-3925**).

5.4.2 *Point Kernel Methods*—Point kernel methods are used mainly for photon transport problems (**~~40~~26**). In point kernel methods, the radiation source volume is approximated by a number of isotropic ~~point sources.~~source points. The absorbed dose at each dose point is obtained by summing the dose contribution from all source points. The calculation takes into account the distance between the dose point and the source point and approximates the scatter within the intervening product through the use of a build-up factor. Build-up factors are theoretically calculated and sometimes fitted to empirical functions. These factors provide an approximation for the contribution of scattered photons from surrounding material. Approximations are also required to account for the energy spectrum and variations in the atomic number in different intervening or scattering materials.

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

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

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

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

5.4.6 The accuracy of the point kernel treatment may be comparable to that of a Monte Carlo calculation for configurations where the point kernel approximation is valid (**~~41~~27**).

5.5 *Empirical and Semi-empirical Methods:*

5.5.1 *Empirical*—Empirical methods typically involve fitting analytical functions to experimental measurements (or to calculations using other methods). The model equations are typically specific to a particular radiation facility and their predictive capabilities are not generally transferable to other facilities or products. Some simple equations exist for calculating the range of electrons in condensed matter (**~~42~~28**), electron energy loss (**~~43~~29**) and depth-dose relationships in various materials (**~~44~~30**).

5.5.2 *Semi-Empirical*—These are empirical methods in which the fitting parameters are constrained so that the model satisfies one or more physical laws or rules. These methods provide a more generally applicable mathematical model than the empirical method and are adjustable to physical parameters of the facility, source and products, such as energy, density and composition. In general, these are software-based programs with variable parameter inputs. Equations, codes and databases are available (**~~45~~-31-34~~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~~ or irradiation applications, or both, that were not part of the original database used to generate the model. These methods may be difficult to implement for systems with complicated geometry.

NOTE 8—~~If a one-dimensional model such as the semi-empirical EDMULT code (~~Although empirical or semi-empirical codes may give~~A1.9, (~~some~~47)) is used to obtain an estimate of the dose in a system that is finite in more than one dimension~~ useful guidance, modern Monte Carlo codes on modern platforms are often very fast in these types of applications. (~~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.~~dose measurements.

6. Prerequisites for Application of a Mathematical Method

6.1 *Facility and Related Geometry Considerations:*

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

NOTE 9—Fig. 1 shows a ~~solid~~physical model of a typical gamma irradiator with product in aluminum totes. For clarity, four totes and part of the source shroud have been removed. The tote irradiator uses a shuffle-and-dwell concept. Each product tote is irradiated for a defined period of time before ~~each tote~~ it is ~~indexed~~moved to the next irradiation ~~positions.~~position. The source rack containing the radiation sources is shown (~~5~~336).

NOTE 10—Fig. 2 shows a photograph ~~of~~ on the left of a research carrier and the graphical user interface window of a mathematical ~~model.~~ model shown on the right photograph. All product is contained in aluminum totes. For the research carrier, product is brought into the ~~irradiator~~ radiation chamber and irradiated for a defined period of time, and then leaves the irradiation chamber. The graphical user interface shows ray tracing between the radiation source (1) and the dose volume (2) (~~5~~336).

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

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

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

6.2 *Personnel*—Trained personnel should be involved in all aspects of model development, program execution, data reduction and the evaluation of results. There is no standard set of qualifications that can be recommended. Interaction of personnel with all

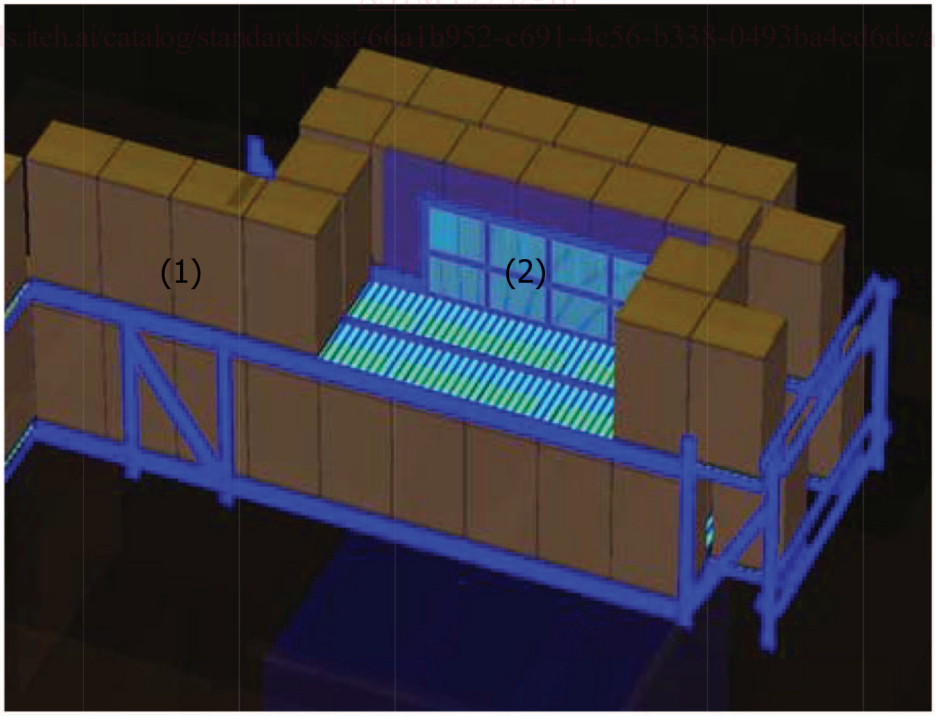

FIG. 1 Solid Model of a ~~Gamma Production Irradiator~~ modified Nordion JS9600 Irradiator with a two layer roller conveyor, showing the product totes (1) and the radiation source (2). The model was developed using EGSPP (~~5~~335)

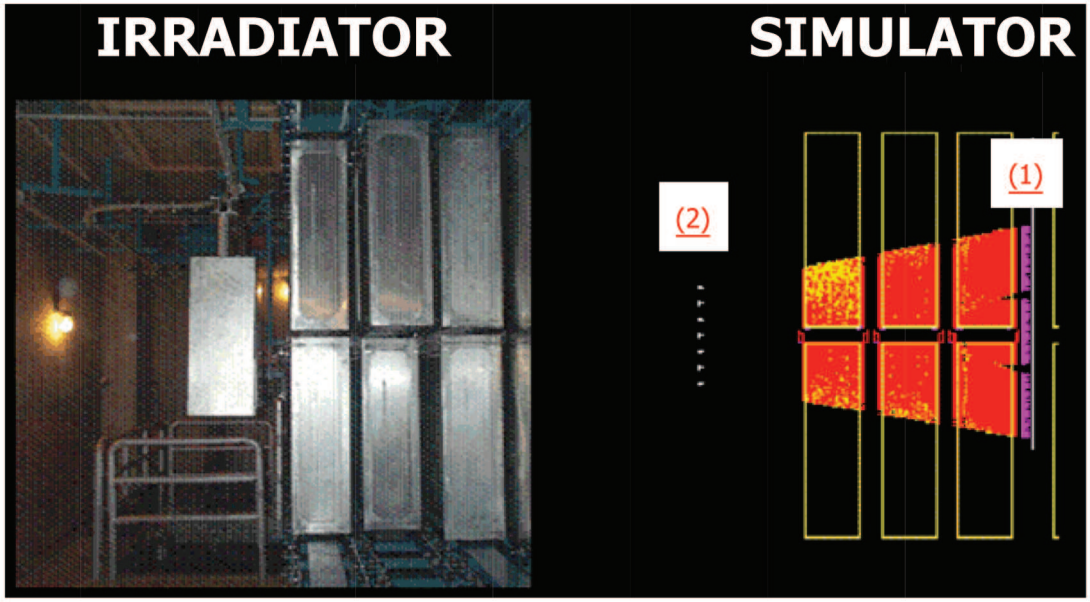

FIG. 2 Picture and Simulation of a Gamma Production Irradiator and Research Loop (~~5~~336)

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.~~recommended since the point kernel method assumes that the energy of the interacting particle is delivered at a point and then distributed statistically around that reaction point, as in the case of photons. On the other hand, electrons interact continuously with matter along their path and because of this the point kernel method is not appropriate.

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

7.2.2.1 Available software may have geometry replication and tiling features that are very useful for this purpose. If the target size is small relative to geometry or source description, Monte Carlo may require biasing or modification to include a larger volume wherein the dose will be an average value over a larger volume than desired. The Monte Carlo method can be used to provide a

refinement of the point kernel build-up calculation to achieve the required accuracy with the point kernel method for optimized efficiency (time, resolution) (**~~41~~27, ~~54~~37, ~~55~~38**).

7.2.3 *Set-up Time*—The ~~complication~~complexity of three-dimensional problem descriptions in the input files and manipulation of the output files is where most of the effort is concentrated and can be very time consuming. It may also be necessary to make modifications to the code to accommodate the specific problem to be solved. If modifications to the code are necessary, revalidation will be required, particularly if the physics modeled in the code has been changed.

7.3 *Selection of Method Type:*

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

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

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

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

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

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

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

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

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

8. Verification and Validation of Model Performance

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

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

8.1.1.1 There are a limited number of referenced benchmark examples in the literature and these may be inadequate in number to validate a method and inadequate in detail for comparison with the model under consideration. The model of the application of interest should be as nearly the same as possible to the benchmark example. Benchmark examples may be found in Annex A5. An example comparing the results of several methods (Monte Carlo, deterministic and semi-empirical) with dosimetry can be found in Ref (**~~56~~39**).

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

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

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

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