

Review of Monte Carlo Modelling Codes

**The Panel on Gamma and Electron Irradiation
Modelling Working Group**

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1 Scope

The Irradiation Panel's Modelling Working Group has reviewed a range of Monte Carlo modelling codes, from the perspective of the industrial irradiation business. This document is primarily intended for potential modellers of industrial irradiation processes, whether they are gamma, e-beam or X-ray. It strives to inform the potential user of some of the strengths and weaknesses of a range of Monte Carlo codes in order to try and simplify the process of selecting an appropriate code.

A selection of six codes has been included: EGSnrc, egspp, Geant4, MCBEND, MCFANG & MCNP. Consideration has been given to a range of features such as ease of geometry input, visualisation capabilities and cost. This report aims to arm the potential user with some basic information on each code, to facilitate an initial choice of the code most suited to their requirements.

Note that whilst every effort has been taken to check the information given in this review, accuracy cannot be assured. For convenience, a number of web links direct to web site pages have been included. These were live at the time of publication, however given the nature of the internet, the sites listed may well change over time.

2 Introduction to the Monte Carlo Method

The Monte Carlo method is one of the most powerful modelling techniques currently available for dose rate/shielding calculations. At its most basic level, the concept is simple even though the software codes used to run the calculations are very complex.

The capability to calculate absorbed doses with the Monte Carlo method offers plant operators a tool that may assist in:

- Prediction of doses that will be received by products, in order to assist with product scheduling or the assessing of new products.
- Assessment of the impact of packaging changes or a revised product packing pattern.
- Reviewing the effects of a new cobalt loading in a gamma plant, before Operational Qualification is run.
- Assessment of the impact of an unplanned change to the irradiation process, e.g. multiple stoppages during a gamma plant irradiation resulting in multiple transit doses as the source rack returns to the safe position each time.
- Designing an irradiation plant, aiming for optimal efficiency and dose uniformity.

2.1 Monte Carlo in principle

Monte Carlo simulations are calculations involving realistic simulations of modelled physical systems, and are used in many areas of physics and chemistry but are of particular importance in the modelling of radiation transport. Particles are created according to rules which determine their type, energy and initial direction. Their interactions with electrons and nuclei within the material of interest are followed according to probabilistic functions using random numbers, which allow the complete history of a particle to be followed as it loses energy within a simulated medium,

perhaps generates other particles, and ultimately is ‘killed’ as it either escapes from the geometry of interest or its energy falls below a given threshold. It is this use of probability functions and random numbers, which gives the Monte Carlo method its name.

Repeated many times, this allows quantities of interest such as the absorbed dose within a medium, to be calculated. The precision with which the absorbed dose is calculated, increases approximately as $N^{1/2}$, where N is the number of histories calculated within the model. The time required for a particular calculation to be performed, then depends upon the model complexity, the detail or resolution used to model the particle tracks, the required precision of the final result, and the speed with which the computer used can perform complex floating-point operations. Laptop computers available now are significantly faster than even supercomputers were in the 1980s and early 1990s, so calculations giving useful results can be obtained in only a few hours (or even minutes, if using a Grid-based system).

Assuming accurate geometry and material compositions have been entered into the model then, when run for millions or billions of particle histories, the simulation closely represents what actually occurs during an irradiation process.

Shultis and Faw¹ contains a very detailed description of the Monte Carlo method as applied to radiation transport.

3 Other Modelling Techniques

Whilst this report focuses on the Monte Carlo technique, it is by no means the only approach available or appropriate for this industry.

Point Kernel modelling for calculations involving photons, has been widely and successfully used within the industry for gamma shielding and dose rate calculations. Whilst Point Kernel still has an advantage over Monte Carlo in terms of speed of computation, it does not offer the same degree of accuracy in predicting absolute dose rates, nor can it be used for e-beam.

Discrete ordinates codes are also becoming more available, such as Attila from Transpire, Inc. These codes solve the transport equation directly on a grid, using the same techniques as finite element calculations. These codes have the advantage that the quantity required (for expel, absorbed dose) need not be predefined, but can be extracted from the resultant fluxes calculated on the grid points after the calculation is complete.

Note that normalisation to obtain an absolute dose rate may be required, although when correctly applied, Monte Carlo calculations are capable of predicting actual absorbed doses with an accuracy limited only by the physics built in to the particular model.

ISO 11137² has a basic explanation of the two principle types of model and discusses some uses of modelling within the industry. ASTM E2232³ offers an excellent overview of the range of modelling techniques available.

4 Introduction to the Codes

The paragraphs and then tables below give outline descriptions of several of the available and more commonly-used Monte Carlo codes. For more information, readers are referred to the websites and other documentation available.

All of these codes are widely used within their principal markets. Given the relatively small number of codes reviewed, the differences in price and usability of the codes is considerable. Some codes require significant programming knowledge, some do not. Some codes require a knowledge of the physics involved, while with others the physics is already incorporated.

If the codes are suitable for running simulations of the irradiation technology of interest (see section 5.3) then in principle they should also be suitable for modelling both Operational Qualification (OQ) and Performance Qualification (PQ). In practice, the relative ease of coding complex geometries differs between the codes. This might make some of them more suited to PQ, for example, where actual product would need to be modelled. Geometry input has not been investigated at that level of detail for this review, although the Irradiation Panel is undertaking a separate exercise to more fully compare ease of geometry input. When using the method in plant design calculations, of course, the fine detail of particular products is not usually a consideration.

4.1 EGSnrc

EGSnrc is a version of EGS (Electron Gamma Shower) that has been developed by the National Research Council of Canada. It is free for non-commercial use (currently NRC is not charging users at all, but NRC should be consulted if significant commercial use is made either of the code itself or the results of calculations) and there is some support available through the website and user community. EGSnrc is limited to photons and electrons, but it aims to model the physics of these particles very accurately. In fact, the strength of EGSnrc lies in its physics capabilities for high precision modelling, particularly of electrons. However, the geometry input and error checking for EGSnrc is extremely challenging and there are limited visualisation tools available.

Pros: Excellent physics for photons and electrons.

Cons: Difficulty of geometry input.

Web Site: <http://www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html>

4.2 egspp

This is a relatively new development from the National Research Council of Canada which was released with EGSnrc in October 2005. Egspp is not a standalone package, but a library of C++ routines that sit on top of the existing EGSnrc code. They greatly simplify the setting up of the model, especially the geometry which can be created using an intuitive text based approach. The geometry files can be read by a visualisation package which works ‘offline’ so that geometries can be modified and viewed without running any simulations. The code is still new, though, so support from the user base is expected to be limited and some of the documentation is not yet complete.

Pros: Excellent physics for photons and electrons (uses EGSnrc) and ease of geometry input/viewing.

Cons: Relatively new, may contain some bugs; still under development

Web Site: <http://www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html>

4.3 Geant4

Geant4 has been developed through an international collaboration of the high energy physics community. It is open source software, with multiple groups working to develop different parts of the code. Described as a ‘a toolkit for the simulation of the passage of particles through matter’, this highlights two key features:

1. This is an extensive ‘toolkit’ rather than a single program. The use of Geant4 requires some C++ skills to bring the various parts of the toolkit together in a program that will run the simulation.
2. Flexibility and breadth of the physics. Geant4 covers an extensive range of particles and interactions.

The scale of the Geant4 collaboration means that there are several options available for tasks such as geometry visualisation/checking. It is a very powerful package that can be programmed to run interactively, either through a graphical interface or the command line, with changes being made to the model parameters. Macros are also available to allow parameters to be changed recursively e.g. to simulate moving objects. The power and scale of Geant4 is, however, both its strength and its weakness:

Pros: A powerful package with the scope to run moving, interactive, graphical simulations of industrial irradiators.

Cons: The initial learning curve for Geant4 is steeper and higher than any other code reviewed here. Some knowledge of C++ is essential as everything must be programmed and there are few shortcuts readily available. A fairly detailed knowledge of the physics being modelled is also required.

Web Site: <http://geant4.web.cern.ch/geant4/>

4.4 MCBEND

Both MCBEND and MCFANG differ quite significantly from the other codes reviewed here in that they are fully commercial packages. These packages have been developed to meet the needs of the nuclear industry and are maintained and distributed by Serco Assurance. Serco Assurance also provide a contract modelling service.

Serco offer a comprehensive package encompassing the software license, phone line technical support and extensive documentation. Data input for MCBEND is relatively simple, with all data contained in one single input file. This is a similar approach to MCNP (see section below) but it also supports the use of names for labelling geometry objects, making it more intuitive. These install as standard software packages and no programming knowledge is required. Comprehensive geometry visualisation and error checking packages are also available.

Pros: MCBEND offers a complete package including geometry visualisation and error checking. It requires no programming knowledge and the physics options are built-in.

Cons: The support and development overheads are higher for fully commercial software and this is reflected in the cost.

Web Site: <http://www.sercoassurance.com/ANSWERS/>

4.5 MCFANG

MCFANG has not been tested for this review, however most of the features are common with MCBEND. The key difference of relevance to the irradiation industry is that MCFANG does not model electrons, either as sources or those arising from ionisation events. Instead, the energy is deposited at the point of the interaction.

Pros: A slightly cheaper option than MCBEND.

Cons: Photons only: no electron physics.

Web Site: <http://www.sercoassurance.com/ANSWERS/>

4.6 MCNP

MCNP is a well established code that has been developed by Los Alamos National Laboratory in the USA. The development of this code split at version 4, branching into MCNP5 and MCNPX. MCNPX has, essentially, been redeveloped to model a wider range of particles and energies. MCNPX has not been included in this review although many of the features are common to both codes.

At the time of testing, MCNP5 was not available for distribution through the European NEA data bank and version 4C2 has been tested.

Like MCBEND, all MCNP data input is in a single file and no programming skills are required. MCNP4 includes a 2D geometry viewer that can also check for geometry errors; MCNP5 also includes the 3D Visual Editor suite of tools. Geometry objects are defined by intersecting surfaces which offers flexibility, however objects are referred to by numbers not names. Physics options can be modified but the defaults will suffice for most applications. The single data output file includes a range of statistical checks, with pass/fail criteria, to help judge the validity of the calculations.

Pros: MCNP is well established and requires no programming knowledge.

Automatic statistical checks on the results will benefit users who are new to the Monte Carlo technique.

Cons: Geometry input is made more difficult by the requirement to refer to objects by number.

Web Site: <http://mcnp-green.lanl.gov/index.html>

5 Code Comparison Tables

5.1 Basic Code Details

	EGSnrc	egspp	Geant4	MCBEND	MCFANG	MCNP
Available from	National Research Council Canada	National Research Council Canada	CERN	Serco Assurance ANSWERS Software Service	Serco Assurance ANSWERS Software Service	USA - Radiation Safety Information Computational Center (RSICC): http://www-rsicc.ornl.gov/ Outside USA – NEA Data bank: http://www.nea.fr/
Version Tested	v4.2.2	(included with EGSnrc)	v7.1	10A	Not tested	4C2
Web site	http://www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html	http://www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html	http://geant4.web.cern.ch/geant4/	http://www.sercoassurance.com/ANSWERS/	http://www.sercoassurance.com/ANSWERS/	http://mcnp-green.lanl.gov/index.html
Brief License Details	Free of charge only for non-commercial research or educational purposes. Written consent is required if the code is to be used for a commercial product or service. In practice at the time of writing, NRC is not charging.	Open source software (GNU GPL), however egspp requires EGSnrc.	Open source. The Geant4 web site has a license page, however at the time of writing only a disclaimer was posted. http://geant4.web.cern.ch/geant4/support/license/index.shtml	Annual, single processor license fee of the order of £20k; 2D & 3D visualisation packages available at approx £3k each.	Annual, single processor license fee of the order of £16.5k. 2D & 3D visual packages available at approx £3k each.	The NEA data bank imposes restrictions on the use of the software: http://www.nea.fr/html/dbprogram/restrictions.htm RSICC license details, for both single user and multi user licenses, can be found at: http://www-rsicc.ornl.gov/rsiccnew/license.pdf The cost of obtaining a copy of MCNP differs significantly depending on the user's country: <ul style="list-style-type: none">• USA through RSICC - single user license \$800.• France via NEA data bank – free• In the UK a full annual access fee to the NEA data bank, administered through NPL, is required. Costs are currently:

	EGSnrc	egspp	Geant4	MCBEND	MCFANG	MCNP
						<p>£5k for companies with an annual turnover less than £50M £10k for companies with an annual turnover greater than £50M. Users from other countries should contact NEA for the costs of accessing the databank.</p>
Level & Type of Technical Support Offered	Some support is offered through contact details on the web site. Users can subscribe to the EGS listserver, a low volume discussion group (mailing list), for update/patch announcements, and to ask questions which may be answered by other users or by the writers.	See EGSnrc	Support section of the web site contains training materials & FAQs. A user forum provides access to developers & users.	Comprehensive technical support is available by phone/email. There is an annual seminar where updates are reviewed.	As for MCBEND.	Los Alamos National Laboratory offers limited, free, technical support. The MCNP web site hosts a listserver forum with a searchable archive.
Documentation	An extensive series of manuals are installed along with the program and are also available from the web site. http://www.irs.inms.nrc.ca/EGSnrc/documentation.html	Limited documentation is currently available as a user manual. A developers manual is promised but has not yet been released. http://www.irs.inms.nrc.ca/EGSnrc/documentation.html	Extensive documentation is available on the web site. http://geant4.web.cern.ch/geant4/support/userdocuments.shtml	Comprehensive user manual, available as pdf or hard copy.	As for MCBEND.	Comprehensive manuals. The MCNP5 manual is now in three volumes: Overview, User's Guide & Developer's Guide. The overview (Volume 1) is available on the website http://mcnp-green.lanl.gov/manual.html

Examples ¹	Yes	Yes	Yes	Yes	As for MCBEND.	No
Training	NRC hold courses on EGS approximately every 1-2 years.	As for EGSnrc	Regular training courses (approx 1-2 per year) are held in global locations. Many of these are free to attend. There is an annual conference plus Geant4 workshops relating to specific topics (http://geant4.web.cern.ch/geant4/pastevents.shtml)	Both introductory & advanced courses are offered. Courses may also be tailored to a particular application. NB - Serco Assurance are offering free training places (for a maximum of 3 people) on the standard Introduction to MCBEND Course, with each MCBEND Licence leased by a member of the Irradiation Industry.	As for MCBEND.	Regular introductory & advanced courses are held globally, although mainly at Los Alamos National Laboratory. Courses now use MCNP5.
User community	There is an active user community, mainly academia based. Much use of EGSnrc is also made within the medical physics community for radiotherapy and diagnostics calculations.	Limited at present.	Extensive, worldwide, mainly academia based. Much use of Geant4 is also made within the medical physics community for radiotherapy and diagnostics calculations.	Users are predominantly based in the UK/European nuclear industry. Networking with other users is possible at the annual seminar.	As for MCBEND.	Extensive, worldwide. MCNP is already used within the irradiation industry.

5.2 Prerequisites

	EGSnrc	egspp	Geant4	MCBEND	MCFANG	MCNP
Hardware requirements (PC only listed)	No specific requirements	No specific requirements	No specific requirements	Pentium III, 128 MB RAM (256 recommended)	As for MCBEND.	Pentium II, 128 MB RAM. Minimum 70 MB hard disk space; complete installation requires 2.3 GB.
Operating System	Linux / UNIX / Windows	Linux / UNIX / Windows	Linux recommended but can be run under Windows via cygwin. <i>NB: Most tools/graphics tend to work best under Linux UNIX although a number of tools (e.g. JAS3) are written in platform independent languages (e.g. Java).</i>	Linux / UNIX / Windows	Linux / UNIX / Windows	Linux / UNIX / Windows

¹ Some codes include example problems that can be modified and run. This can be an effective way of learning how to use software features.

Programming languages	Knowledge of Mortran is required. Knowledge of FORTRAN helpful.	Whilst no specific programming skills are required, some knowledge of C++/Mortran/Fortran or even a basic scripting language would assist in setting up complicated plant geometries.	Basic knowledge of C++ essential.	No programming required.	No programming required.	No programming required.
Essential Additional Software Required	None	None	Windows implementation requires C++ compiler e.g. Microsoft Visual C++ Express version (free) plus windows platform software development kit (free) <i>NB: You can run under windows using cygwin/g77 (i.e. without Visual C++) but this is not the 'official' way to do it.</i>	2D (VISAGE) and/or 3D (VISTA-RAY) visualisation/geometry checking packages highly recommended.	2D (VISAGE) and/or 3D (VISTA-RAY) visualisation/geometry checking packages highly recommended.	None

5.3 Applications

	EGSnrc	egspp	Geant4	MCBEND	MCFANG	MCNP
e-beam	Yes	Yes	Yes	Yes	No	Yes
gamma	Yes	Yes	Yes	Yes	Yes; photons only, no electron transport	Yes
X-ray	Yes (No photoneutrons)	Yes (No photoneutrons)	Yes	Yes	Yes; by defining x-ray source directly rather than using electron interactions. (No photoneutrons)	Yes
shielding	Yes (but no neutrons)	Yes (but no neutrons)	Yes	Yes	Yes (but no neutrons)	Yes
photoneutron / product activation	No	No	Yes	No	No	Yes

5.4 Code Technical Details

	EGSnrc	egspp	Geant4	MCBEND	MCFANG	MCNP
Underlying programming language	Written in FORTRAN, with a Mortran front end.	C++ running on top of the EGSnrc FORTRAN/Mortran. NB: Further development is expected to move egspp entirely into C++.	C++ The development of the Geant4 code follows rigorous software engineering practices (http://geant4.web.cern.ch/geant4/OOAandD/index.html)	FORTRAN	FORTRAN	C++ front-end on a FORTRAN back-end.
Physics	electrons/photons <ul style="list-style-type: none"> Extremely good physics for electrons/photons. Generally, calculations can be run with all of the physics options active by default so, whilst some parameters can be adjusted, it is not normally necessary to do so. Cannot handle neutrons e.g. photoneutrons generated in high-energy X-ray facilities. 	Same as EGSnrc	All relevant particles <ul style="list-style-type: none"> Need to build in user's choice of physics, however the standard electromagnetic physics package would suite most applications. Extensions available to low energies (i.e. MeV region downwards) which are becoming more accurate as users add improvements. Individual physics objects are under complete user control and new ones are being developed continually by the user community. Can be used for shielding calculations where photoneutrons are generated for example in high-energy X-ray facilities. 	electrons/photons/neutrons <ul style="list-style-type: none"> Physics is built-in for electrons, photons and neutrons. Variance reduction/acceleration is accommodated. Neutron data available from most of the standard evaluated nuclear data files. 	photons/neutrons <ul style="list-style-type: none"> NB – MCFANG does not have electron tracking. If an ionisation event occurs, the energy is dumped at the photon interaction point. MCFANG is 'multigroup'. Whilst MCBEND calculates or looks up cross-sections explicitly for energy, the multigroup approach uses a series of average values over ranges of energies. 	electrons/photons/neutrons <ul style="list-style-type: none"> Physics is built-in for electrons, photons and neutrons. Can adjust parameters (such as cut-offs) as required. Can be used for shielding calculations where photoneutrons are generated for example in high-energy X-ray facilities.
Radiation Source Definition	Source geometries and spectra need to be explicitly defined, independently of the materials geometry.	Same as EGSnrc	Sources and spectra need to be explicitly defined, independently of the geometry.	Sources in MCBEND can be defined in several ways: <ul style="list-style-type: none"> as previously defined geometry objects as sources independent of geometry by material. 	As for MCBEND.	Sources and spectra need to be explicitly defined, independently of the geometry.

Energy Range	1keV - 10 GeV	Same as EGSnrc	~250eV - 100 TeV (for electromagnetic processes of interest in this work). Photonuclear physics starts at 10 MeV.	10 keV – 14 MeV	10 keV – 14 MeV	1 keV – 100 GeV (photons) 1 keV – 1 GeV (electrons)
Validation / Benchmarking	The EGSnrc distribution includes document, NRCC Report PIRS-703 describing QA tests. Many other references exist describing benchmarking tests including for the critical radiotherapy applications.	As for EGSnrc at least as regards physics; eg spp is too new to have significant industry benchmarking as yet for other applications.	Significant documentation exists and is being added to by the Geant4 collaboration including for the critical radiotherapy applications. http://geant4.web.cern.ch/geant4/results/results.shtml	MCBEND is validated for an extensive range of applications. The validation database covers many of the materials and geometries that are encountered in the nuclear industry. Gamma ray benchmarks cover scatter and reflection of gamma rays as well as penetration through shield materials. http://www.sercoassurance.com/ANSWERS/resource/area	No benchmarking validation to date.	Significant documentation exists including for the critical radiotherapy applications. http://mcnp.green.lanl.gov/publication/mcnp_publications.html

5.5 Data Input

	EGSnrc	egspp	Geant4	MCBEND	MCFANG	MCNP
GUIs	Some configuration and the setup of a run can be done using a GUI.	Same GUI used as for EGSnrc.	The MOMO GUI combines facilities for geometry viewing and running. There are many tools available for Geant, however the primary method of working is by programming code. GUIs can be created for each application.	A GUI called Launchpad offers some functionality to load files, launch text editors and run simulations.	As for MCBEND.	Visual Editor is included with MCNP5. This has not been reviewed, however the website describes it as a GUI including the following capabilities: <ul style="list-style-type: none"> • Creation and display of geometries • 3D visualisation • Plotting of particle tracks http://mcnpvisied.com
Geometry Input	Inputting complex geometries is challenging. All geometries must be defined by explicitly stating the distances between objects and boundaries (HOWFAR and HOWNEAR routines). This is not intuitive.	Geometries and sources defined in text files; complex geometries relatively easy to enter.	<ul style="list-style-type: none"> • Geometry usually entered directly using C++, however geometry design tools (e.g. GGE, part of MOMO) are under development or available. • GDML can be used to describe geometries in a more ‘readable’, portable <i>NB: Objects and materials can be defined by name, not just a number. This makes the file easier to read and</i>	<ul style="list-style-type: none"> • Text-based input for geometry, materials & sources. • All data input is held in one file. <i>NB: Objects and materials can be defined by name, not just a number. This makes the file easier to read and</i>	As for MCBEND.	<ul style="list-style-type: none"> • Text-based input for geometry, materials & sources. • All data input is held in one file. <i>NB: See note under MCBEND.</i>

	EGSnrc	egspp	Geant4	MCBEND	MCFANG	MCNP
			fashion using an XML type language.	<i>interpret than MCNP.</i>		
Geometry Replication	Each object must be specifically defined; objects cannot be defined once and then replicated.	Geometries can be readily translated/repeated or exported to other models.	Geometries can be readily repeated or exported to other models; the object oriented approach of Geant4 naturally lends itself to geometry replication.	Replication of parts within a geometry is supported. It is simple to transfer geometries between different MCBEND models.	As for MCBEND.	Geometries can be replicated and exported, with care.
Geometry Visualisation /Checking	Debugging geometry is difficult; there is no universal geometry viewer. Under Linux, the egs_windows geometry viewer can be used.	<ul style="list-style-type: none"> • 3D Geometry can be easily viewed offline using egs_view under Linux or Windows. Objects/regions can be very simply faded or coloured by choice. • Basic geometry checking available. • Some bugs exist but may be worked around. (Cannot place objects inside a prism geometry; some difficulties with replicated coaxial cylinders inside a geometry.) 	<ul style="list-style-type: none"> • Inbuilt geometry checking commands and external tools such as DAVID are available. • Runtime geometry viewing and verification options. • Geometries can be exported to standard formats such as OpenGL or VRML. Standard software is readily available for viewing these file types. 	<ul style="list-style-type: none"> • 2D (Visage) & 3D (Vista-Ray) visualisation / geometry checking packages can be run from the GUI. • Visage displays 2D slices calculated using ray-tracing. It can also measure geometry coordinates. • Vista-Ray displays 3D images, also ray-traced. • Both packages display region identification information. • Both packages offer geometry checking by searching for multiply defined regions. This can be output to a file or displayed visually. • Both packages can display the radiation source on the geometry model display. 	As for MCBEND.	<ul style="list-style-type: none"> • A 2D viewer is included with MCNP. This offers geometry checking by visually highlighting multiply defined regions within a 2D section; the checking is limited to the section on view. • The 2D viewer will also display particle tracks during a simulation run. • A 3D visualisation package/visual editor (Visual Editor) is included with MCNP5 http://mcnpvised.com Sabrina is an alternative third party package.
Moving Product Simulation	Not possible directly, would have to run successive static simulations with changed geometries. Difficulties with geometry setup/checking would make this difficult.	Not possible directly, would have to run successive static simulations with changed geometries. This is relatively easy using the EGS_Transformation macro to move objects.	Simulation of moving product possible directly through macros. This could also be done interactively during a run.	Can handle movements within a simulation using some parameterisation / looping.	As for MCBEND.	Not possible directly, would have to run successive static simulations with changed geometries.

5.6 Data Output

	EGSnrc	egspp	Geant4	MCBEND	MCFANG	MCNP
Data Analysis	None - basic text output.	None - basic text output.	<ul style="list-style-type: none"> • Geant4 provides some analysis options including statistical analysis (e.g. JAS3). • Supports AIDA interfaces which enables other AIDA-compliant analysis tools to be used e.g. OpenScientist. 	None, but you have control over the output format so it can be tailored for your choice of analysis package. <i>NB - Currently it does not provide absorbed dose as an output parameter.</i>	As for MCBEND.	<ul style="list-style-type: none"> • Basic text output. • By default, it performs ten statistical checks on the results indicating pass/fail based on given criteria.

6 Further Information

As well as the web sites for each of the individual codes, there are several publications which are of interest to the potential modeller. ISO 11137² discusses the application of modelling within the irradiation industry. ASTM E2232³ is a more extensive guide to the use of modelling techniques, including Monte Carlo, to calculate absorbed dose. In addition, there is an EC document published by NPL that reviews a range of Monte Carlo codes⁴. Whilst some of the codes have now been upgraded, much of the information is still relevant. Copies of the review are available through the working group or directly from NPL.

RPSMUG (Radiation Process Simulation and Modeling Users Group <http://www.rpsmug.org>) is an organisation advancing the use of mathematical modelling within the irradiation industry. RPSMUG offers training courses and meetings are held at least annually. The web site is a valuable resource for members including an online library, industry news and member contact details.

7 Glossary

GNU General Public License agreement - This is a general open source license agreement that allows the program to be used for any purpose. The program may be freely copied, distributed or modified and the modified version released to the public so long as access to the source code is always given. Programs derived from a GPL licensed program are also encompassed by the GPL license agreement and cannot be distributed as proprietary software.

Listservers - These are open discussion groups. Users can register and then send or receive e-mails to/from all members of the discussion group.

Mortran - an extension of FORTRAN. It introduces syntax changes, including the use of semicolons to end statements, in order to improve readability and flexibility.

Open Source Software - Open source generally refers to software for which the programming code is available and open for inspection, modification and redistribution by anyone. Any code derived from it must also be open source. Whilst open source software is often free, it does not necessarily have to be.

8 Contributors

This document has been prepared by the Modelling Working Group of the Irradiation Panel. Many group members have contributed to the development of this document, and particular thanks are extended to:

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9 APPENDIX A: Simplified gamma irradiation vault modelling exercise

This Appendix describes the geometry modelled using the Monte Carlo codes described above.

It was not intended that this should resemble any real irradiation facility, but that the basic ‘essence’ of such a facility would be captured – the presence of a source rack, the presence of product in rows each side of the source rack, inside a concrete vault. In order to keep things simple, no structures such as entrance/exit labyrinths, conveyor systems, source rack support frames, product-supporting totes or the source storage pool are described here.

The aim was to demonstrate:

- a. For each code used, how much effort is required to code sources (with individually-assigned activities to each source pencil, and including the presence of ‘blank’, inactive pencils), and how much effort is required to code product with dosimeter arrays within them
- b. What steps had to be taken to run the codes, how long the runs took; and finally
- c. How the output could be analysed to provide useful information.

9.1 Radiation source:

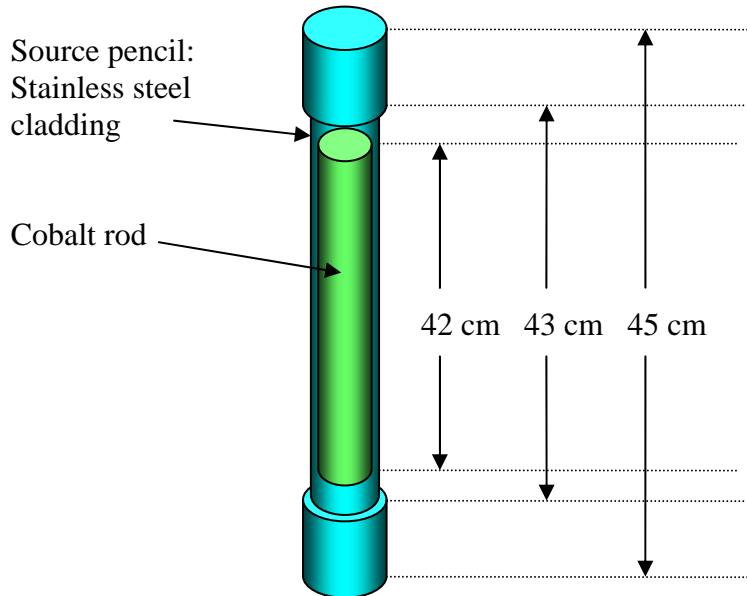
It is important that any model of a commercial irradiator includes a fairly detailed model of the radiation source. In this model, a source rack comprising cobalt-60 pencils in a regular array was used. Such a source rack may typically contain several modules, each of which may comprise several dozen source pencils and some inactive ‘dummy’ pencils.

The source rack for this model, consisted of four modules of 42 source pencils as described below. Supporting steel frameworks were omitted for simplicity. The source activities were individually assigned to each source pencil, in order to investigate the ease of assigning activities to fully-modelled source racks.

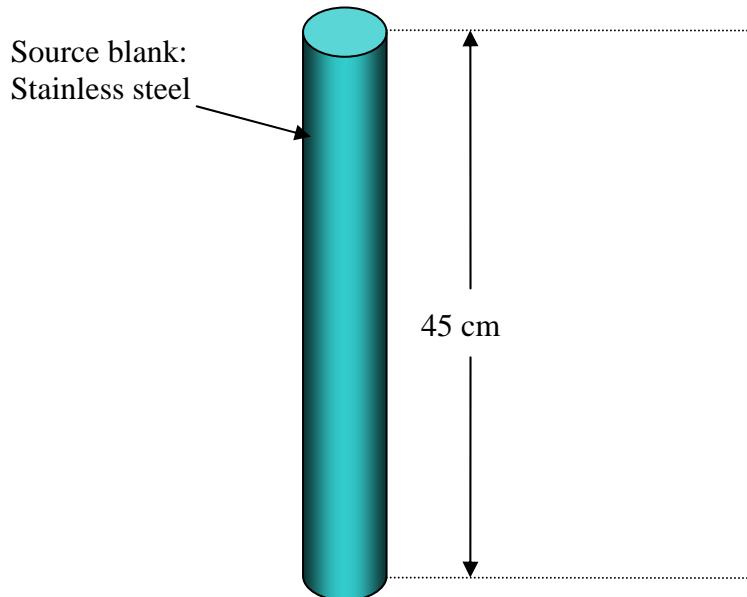
9.2 Source pencil:

A typical source pencil for this model would be a 42.0 cm long, 8.5 mm diameter cobalt cylinder. This was clad in 316L stainless steel, as a 43 cm long, 10.0 mm diameter cylinder. At each end were two 1.0 cm length, 11.1 mm diameter cylinders as end caps, so that the entire pencil was 45.0 cm long. The composition of the 316L stainless steel was 0.7% silicon (by weight), 17% chromium, 1% manganese, 66.8% iron, 12% nickel and 2.5% molybdenum. Its density was 8.06 g cm^{-3} .

The cobalt cylinder within this was treated as normal cobalt, density 8.9 g cm^{-3} .

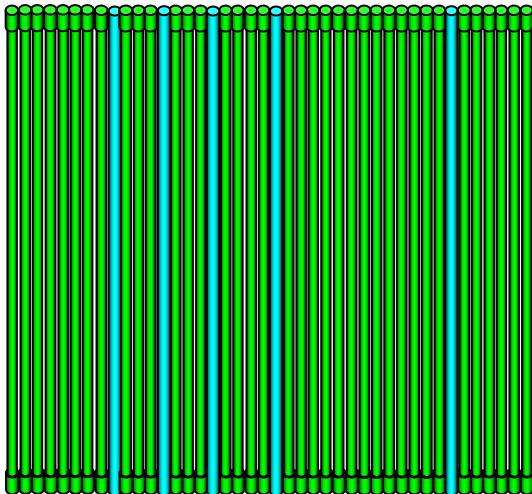


A 'dummy', inactive pencil, is represented as a simple cylinder, 45.0 cm length, 11.1 mm diameter, stainless steel.

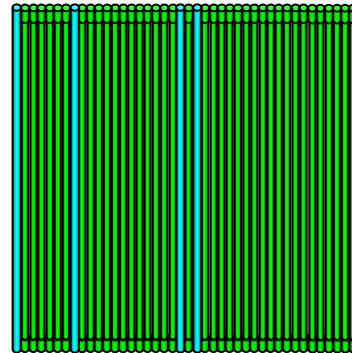
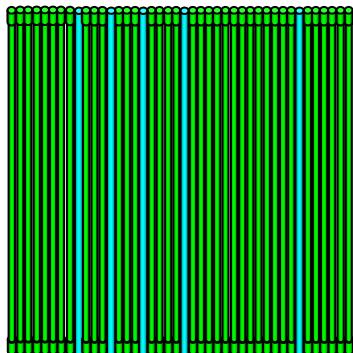


9.3 Source module:

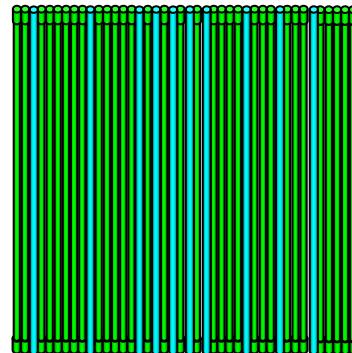
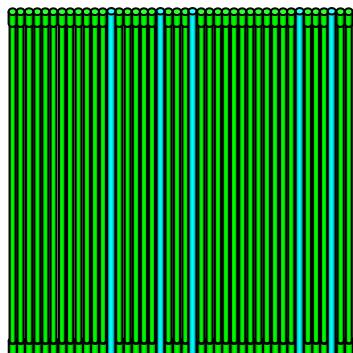
A source module for this model, comprises 42 of the above pencils numbered 1 to 42 from left to right. The illustration below shows such a module, actually the first module for this model. There is no supporting frame in this model of course, but five dummy pencils (blue) are shown among the active ones (green).



9.4 Source rack:



The source rack for this model, comprised four of these modules, in a 2×2 array. The modules were separated by 2.5 cm horizontally and vertically. In this illustration, the source rack is set up as for the actual test geometry.



Source activities:

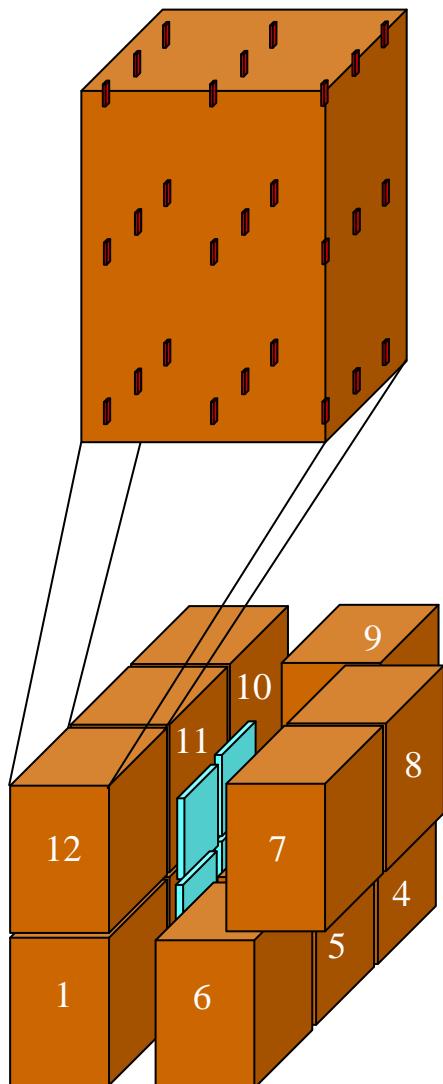
The activity of each pencil was individually assigned, including zeroes for the dummy pencils. The source material is cobalt-60, with two gamma-rays at 1.17 and 1.33 MeV, with the activity normalised so that 1.0 in the activity array corresponds to 1.0 kCi.

The activities are given in the accompanying Excel spreadsheet. The modules within the rack are numbered from 1 to 4, as follows:

1	3
2	4

9.5 Product and dosimeter arrays:

Dosimeters:



Dosimeters were arranged in regular, 3×3 \times 3 rectangular arrays in the product boxes. The individual dosimeters were modelled on Harwell Perspex® dosimeters, and so comprised PMMA (polymethylmethacrylate, $C_5H_8O_2$) of density 1.19 g cm^{-3} , in a volume 3.0 high by 1.1 cm wide (parallel to the source plane) and 0.3 cm deep (perpendicular to the source plane). Dosimeters were placed so that those near the sides of a product box, had their edges 1.0cm inside the product. Absorbed dose was recorded in individual dosimeters, in units of kGy hr^{-1} ; care had to be taken here as these dosimeters are normally calibrated in terms of dose-to-water, and different Monte Carlo codes produce results based on ‘tallies’ which may require further work to convert to this quantity.

Product:

These arrays of dosimeters were arranged in rectangular boxes, 90.0 cm high by 100.0 cm wide (parallel to the source plane) and 60.0 cm deep (perpendicular to the source plane). The ‘product’ comprised water at a density of 0.16 g cm^{-3} . (Note that this does not represent any real product, but is in fact a fairly good approximation to the typical material being irradiated in such facilities.)

The product boxes were arranged in two layers vertically, each group of six either side of the source rack, separated horizontally and vertically by 5.0 cm, and placed symmetrically each side of the central horizontal plane between the two rows of source modules in the source rack. The front faces of the boxes were 10.0 cm from the source rack central plane. A total of twelve boxes were modelled, so three boxes were in each layer of product, each side of the source rack. The illustration above shows the general arrangement, with two boxes moved slightly out of the way to show the approximate position of the source rack. They are numbered here to give nominal dwell positions.

9.6 Irradiation Vault:

The interior of the irradiation vault containing the sources and product, was a rectangular ‘box’ of air, 3.0 metres high. The walls were placed 1.0 metre from the product so the vault interior had a total area 5.1 metres long (parallel to the source plane) by 3.4 metres wide (perpendicular to the source plane). The bottom layer of product was 50.0 cm from the floor, so the central horizontal plane of the source racks and product layers were positioned 142.5 cm above the floor.

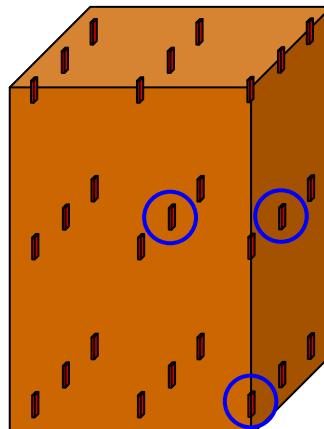
The vault was surrounded by a rectangular ‘box’ of ordinary concrete (hydrogen 2.2% by weight, carbon 0.3%, oxygen 57.5%, sodium 1.5%, magnesium 0.1%, aluminium 1.2%, silicon 30.5%, potassium 1.0%, calcium 5.0%, iron 0.7%, density 2.3 g cm^{-3}), 1.0 metre thick in each direction, so it has overall dimensions 7.1 metres long (parallel to the source plane) by 5.4 metres wide (perpendicular to the source plane) by 5.0 metres high. Again, the concrete specification tested the ease of specification of such a mixture for the codes tested.

9.7 Results:

The results from each codes tested are summarised below.

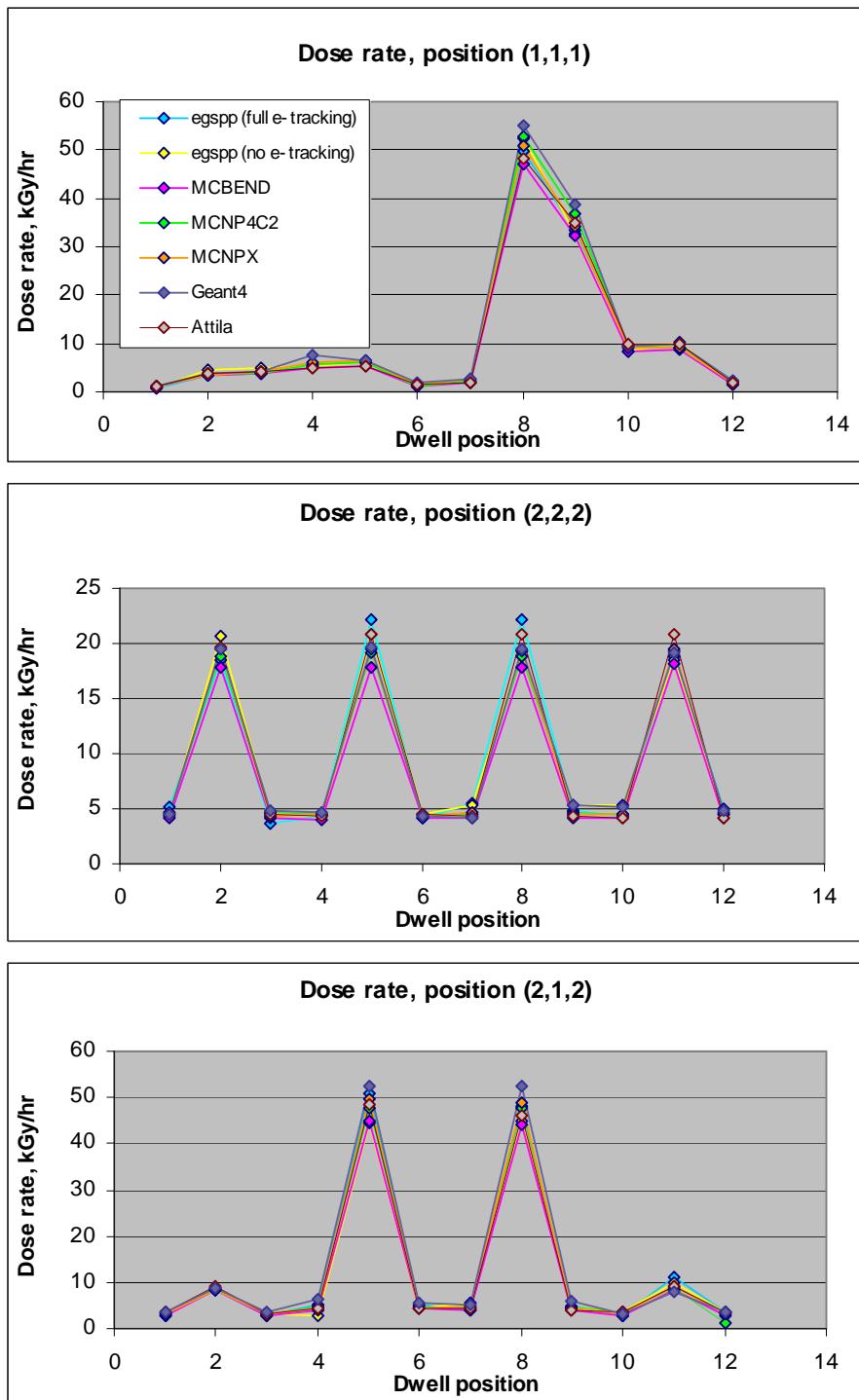
The results are plotted for instantaneous dose rates in the position each box occupied, for dosimeter locations shown here. The average dose rates for all box positions are tabulated.

All radiation transport codes work to solve the Radiation Transport Equation. In Monte Carlo calculations, the regions for which a quantity (say, the absorbed dose) is required are defined in the problem, and the quantity is calculated as the Monte Carlo calculation proceeds. In Point Kernel calculations, the line of sight absorbance between the region the dose is required and the source, is calculated and a scattering kernel added to enable an approximate solution including absorption and buildup via scattering processes to be calculated. In discrete ordinates calculations, the linear Boltzmann Transport Equation is solved directly on the points of a polyhedral grid defined throughout the problem geometry; other required quantities such as the absorbed dose at any required point, are then calculated subsequently, by interpolation of the fluxes calculated at the grid points.



Monte Carlo calculations require time to calculate the results as the accuracy increases statistically as the number of histories is increased. The discrete ordinates approach taken for example by the code Attila, gives results with no statistical noise, and the accuracy is limited by the fineness of the geometric grid defining the problem geometry, and by the details of the multigroup approach taken to the energy spectra in this type of calculation.

Attila is however outside the defined scope of this report and its results are simply included for completeness. More details of this code and its applications may be found at <http://www.transpireinc.com/>.



The above figure shows the dose rates at the locations in the tote described on page 20. The “dwell position” is as described on page 19. Very encouragingly, all the codes used gave dose rates which agreed very well within a few percent.

9.7.1 EGSnrc/egspp:

The geometry was set up with the egspp system. This is a text-based and relatively intuitive method for entering the details of complex geometries for objects and sources, although large and complex geometries do of course lead to large input files of type .egsinp. With many repeated elements, geometries such as source pencils or conveyor rollers are more economically defined using a small computer program to

write that part of the .egsinp file, with the output then simply pasted into the .egsinp file in the appropriate place; this approach has been taken with some of the other codes as well. (This may be done with the Mortran pre-processor language used in EGSnrc, or with Fortran or other interpreted or compiled codes such as Python, C++, or Visual Basic directly, or by using a macro within a spreadsheet such as Microsoft Excel.)

Egspp is available as part of the EGSnrc distribution and is still undergoing development at the time of writing although testing against real dosimetry results in a complex geometry [6] does show that it is capable of delivering extremely good results.

The older EGSnrc system does not benefit from such a geometry interface, and geometries have to be set up by explicitly writing the HOWFAR and HOWNEAR subroutines, and then an additional subroutine AUSGAB for controlling dose deposition and any other required quantities. Writing the geometry subroutines HOWFAR (which returns the distance of the particle under consideration, to the nearest boundary of the current region, in the current direction of travel of that particle) and HOWNEAR (which returns the distance of the particle from the nearest boundary) can be a very complex process, even for simple geometries. Writing the geometry for a complex geometry such as that for a commercial gamma irradiator with this method, is not recommended!

Materials information such as composition, densities, photon and electron cross-sections, are generated in a pre-processor code, PEGS4. This may be run from the EGSnrc GUI (available as part of the EGSnrc distribution) or explicitly from a command line. It takes a fairly simple set of input data (materials to be included, density, minimum and maximum energies for electrons and photons) and produces a large table of output data which is then read in by an EGSnrc or egsspp code during the initialisation process for a given Monte Carlo calculation.

The photon and electron cross-section tables are produced within a user-defined energy range, from a minimum (at least 1 keV) to a maximum (the highest energy available is 50 GeV).

General note: Most measurements of absorbed dose are traceable to a National Standard which is calibrated in terms of absorbed dose to water (in fact, usually absorbed dose to water in a beam of photons from ^{60}Co). A small adjustment (about 3%) should therefore be made using the stopping power ratio between water and Perspex, to give the absorbed dose to water recorded in the Perspex dosimeters. When calculating the doses delivered to other materials, the appropriate stopping power ratio should be used. Alternatively, when calculating the doses recorded in dosimeter volumes, these can be specified with water as the material of interest.

9.7.2 MCNPX / MCNP4:

MCNPX is capable of following many different types of particle through a geometry, in contrast to codes such as EGSnrc which is targeted towards photons and electrons or positrons. MCNP4 is an older variant of the MCNP code; it can follow photons, electrons/positrons, and neutrons through a system.

Both MCNP4 and MCNPX use a ‘combinatorial geometry’ approach, where surfaces are set up and then combined together to create volumes, which are then filled with each required medium. These volumes are entered as ‘cards’ with a series of numbers;

this is not intuitive to look at or enter, but very economical in terms of the input volume required. Commenting these input ‘decks’ is therefore vital, as otherwise it is not clear what any given line describes. (The user manual for MCNP4 has been described as being quite difficult.)

Repeated structures are easily generated using either the older MCNP4, or the newer MCNPX. The particular geometry described in this document uses a number of repeated structures, for example, the source pencils, the source modules, the dosimeter volumes within a tote, and the totes themselves.

Materials may be effectively defined as compounds (elements combined by atomic fractions, so PMMA or water for example) or as mixtures (elements combine by weight fraction, such as with concrete). They are entered into volume elements with their densities assigned at that point.

Scoring for these examples was carried out via either the F4 tally which scores dose using the kerma (kinetic energy released per unit mass in a beam of uncharged particles such as photons) approximation, or the F6 tally which scores MeV/gram in the scoring region directly from the slowing down of charged particles. This requires understanding of the basic physics here so that for example the relationship of absorbed dose to kerma is understood. The F4 tally is scored in terms of rads per source photon in PMMA.

To give a dose map over a whole box, a ‘mesh tally’ was also used with the MCNPX example where the dosimeters were not needed. This facility represents an advantage of MCNPX over some other codes.

It should be noted that there is a subtlety in the setup required for use of the F6 tally so that the materials used need to be entered as percentage masses, not as molecular ratios; this is in contrast to how the materials are set up for tracking the particles of interest. It has been observed that misunderstanding the application of different MCNP tallies is a common source of error. This clearly indicates the importance of appropriate validation of the models used (and this is true, for whichever mathematical model is used, whether Monte Carlo, Point Kernel, or Deterministic).

Finally, there is a limit on the total number of detectors which can be assigned in MCNP4, so that the geometry had to be run a number of times to build up the full matrix of doses recorded in the dosimeters. This limit is not present in MCNPX.

9.7.3 MCBEND:

Geometry input for this code is based on a ‘fractal geometry’ system, whereby objects are combined together using clusters, nests and arrays. ‘Clones’ are used to generate replica geometries. The geometry input is comprehensive, and fairly intuitive. Data entry ‘cards’ are simple, one line for each element in most cases, so repeated elements are economical to enter and easy to check.

Materials are set up in a two-step process, setting up the chemical makeup of mixtures for example, first, and then combining these materials into the volumes as necessary and assigning densities.

Sources in this case are set up in terms of becquerels per unit volume, so this needs to be calculated from the known source strength and volume. This source is then applied to a whole geometry unit comprising a source, so in this case you would have 42

source strengths for the source pencils, and then a zero for the activity of the air box containing those pencils.

Scoring is done using fluxes, so it is important to know how the fluxes may be converted via kerma to absorbed dose (in this case in kGy per hour).

Note that in this calculation, electron tracking was switched off.

9.7.4 GEANT4:

Geant4 is a 'toolkit' for the simulation of all types of particles through arbitrary materials and geometries and includes a wide variety of physics models and processes. For this application, Geant4 v9.0 was used with the low energy physics package which includes all the relevant electromagnetic physics models and processes for the simulation of gammas, electrons and positrons down to $\sim 250\text{eV}$. Hadronic processes are not required in this application and so were not enabled. The default threshold for the production of all secondary particles was set (in terms of distance travelled in a given geometric region) to be 1mm in all regions except in the dosimeter regions where a cutoff of 0.1mm was used.

Geometry in Geant4 can be defined in a number of different ways (see earlier in Section 5.5). For this application, the geometry was relatively simple and so was explicitly defined in C++ by creating a new class derived from a DetectorConstruction abstract base class. Many types of solids (CSG, BREP etc) can be easily defined and positioned in Geant4 using the built-in base classes and replication/repetition of these can be easily achieved. Totes and dosimeters were positioned by repeatedly placing a single defined base volume. Similarly, the source rack was setup by defining the location of the first source pencil in each source module and then repeatedly placing the remaining pencils in the module at a fixed distance from the previous one.

Material definitions and the assignment of materials to volumes were performed when defining the base volumes. Any form of material can be created and usually involves first defining the elements and/or isotopes in the material and then combining them to define the required molecule or mixture (in terms of the fractional mass of each component).

The different source strengths were modelled by defining a suitable cumulative probability function (CPF) based on the tabulated source activities of the 4 modules into the source generator class (PrimaryGeneratorAction). This CPF was then used to determine the particular source pencil producing the initial photon together with the other initial source parameters (such as the random position within the active volume of that pencil).

Scoring was achieved by explicitly writing code in the user action class G4UserSteppingAction to record the energy deposited by the particle track as it crosses a dosimeter region. This class provides access to the particle step parameters and the energy deposited during a step in a given region can easily be recorded (in a similar way to the AUSGAB routine in EGS). More recent versions of Geant4 now provide a number of primitive scoring classes that allow a variety of track-length and deposited-energy based parameters to be scored in a given volume. These classes provide a more straightforward solution to the scoring of dose in a given region.

9.8 Conclusions

All the codes tested gave results, which when compared with each other, were in good agreement within a few percent. Confirmation of the general quality of the results can be obtained by consulting some of the references to ASTM 2232 [3] or for example by reviewing references [5,6]. In these papers, the results of the calculations are compared explicitly with high-precision dosimetric measurements.

Any of these codes would be suitable for use in modelling given situations, although some are more expensive to acquire than others. All however require experience and a physics background in their use, and appropriate care in terms of commenting and validating the input files (geometries for materials and sources) is strongly urged.

10 References

- ¹ ‘Radiation Shielding’, J. K. Shultz and R. E. Faw, Prentice Hall, 1996.
- ² ISO 11137-3:2006, ‘Sterilization of health care products -- Radiation -- Part 3: Guidance on dosimetric aspects’, Annex A
- ³ ASTM, 2002. ASTM International, ‘Guide for Selection and Use of Mathematical Methods for Calculating Absorbed Dose in Radiation Processing Applications’, ASTM E 2232 (ASTM International, West Conshohocken, PA, USA)
- ⁴ H. Tagziria, ‘Review of Monte Carlo and Deterministic Codes in Radiation Protection and Dosimetry’, published by National Physical Laboratory (2000). ISBN 0946754322
- ⁵ J.P. Sephton, P.H.G. Sharpe, R.D.H. Chu, K.P.J. O’Hara, A. Abdel-Rehim, A. Abdel Fattah. ‘Dose mapping of a ⁶⁰Co industrial irradiation plant using an electronic data recording system, static measurements and mathematical modelling.’ Rad Phys Chem 76 (2007) 1820 – 1825
- ⁶ M. Bailey, J.P. Sephton, P.H.G. Sharpe, ‘Monte Carlo modelling and real-time dosimeter measurements of dose rate distribution at a ⁶⁰Co industrial irradiation plant’, Rad Phys Chem 78 (2009) 453 – 456