Directional Spectrum Model for Phase Space Modelling in Monte Carlo Simulations for a Medical Linear Accelerator in Radiotherapy

by

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To Louise, my wife

Without her, this thesis would not be possible.
Abstract

Cancer is the number two killer after cardiovascular diseases according to the World Health Organisation. It is generally accepted that about 50–55 % of all cancer patients benefit from radiotherapy treatment in which high-energy photons from medical linear accelerators (linacs) are commonly used. It is the goal of 3D conformal radiotherapy and intensity modulated radiotherapy (IMRT) to maximise the radiation dose to the tumour site while minimising the dose to the surrounding normal tissues. Thus the radiation beam is shaped to conform to the tumour outline by the multileaf collimator (MLC). Fast and accurate dose calculation is essential to the success of the treatment. The current method of choice is the superposition/convolution method for its computation efficiency but the complexity of the algorithm grows as the treatment moves into complicated regimes. The Monte Carlo method, on the other hand, uses one algorithm for different treatment regimes and its accuracy has been well proven. The drawback of the Monte Carlo method is in its computationally intensive and time-consuming nature.

In a Monte Carlo simulation of a linac, it is common practice to divide the process into steps so that duplicate simulation of the patient-independent components can be avoided. Furthermore, the data of all particles emerging from any linac component form a phase space. A summary of these data allows, in principle, the generation of unlimited number of particles for simulations downstream. This summary is known as phase space model. This thesis examines different phase space models generated from the simulation of the patient-independent components. Under investigation is the 6 MV beam from the Elekta SLi linac.

Two well-known phase space models, the point source model (PSM) and the multiple source model (MSM), were successfully implemented with MCNPX version 2.4.0. A new model termed the directional spectrum model (DSM) was
proposed. In contrast to the PSM and the MSM which loosely relate the particle energy to its direction, the DSM couples the energy spectrum directly to the flight direction so that the scattering properties in the linac head are well accounted for. The DSM calculated dose distributions compare favourably with measurements in water phantom. It performs well inside and outside the 5×5, 10×10 and 20×20 cm² fields. The confidence limits are generally within the American Association of Physicists in Medicine recommended tolerance of 2 % on central axis (CAX) beyond the depth of maximum dose ($d_{\text{max}}$) and 3 % in other low dose gradient regions. The shifts in the high dose gradient regions are also within the recommended tolerance of 2 mm. These shifts were measured in the dose build-up regions before $d_{\text{max}}$ and in the isodose curves in a diamond-shaped field. The DSM also performs satisfactorily in the dose profiles formed by a single leaf of the MLC in a large field. After convolution with a Gaussian kernel, near perfect matches were obtained between the DSM calculated profiles and the R<sub>K</sub> chamber measured ones.

Since statistical fluctuations are unavoidable in any Monte Carlo calculations, denoising techniques from the image processing community could be invaluable tools in smoothing out the statistical noise in the dose distributions. The two digital filters assessed in this work are a Gaussian filter and a median filter. The median filter preserves the beam edges better than the Gaussian one. The smoothed isodose curves also have shifts within the recommended tolerance.

This study indicates that the DSM, possibly together with denoising techniques, is a good candidate for IMRT calculations. Further studies should be carried out to confirm the DSM performance over a wider range of assessments including the modelling of higher energy linacs.
Acknowledgement

Working towards this PhD degree has brought me much joy; finishing it is a tremendous satisfaction. I am very much in debt to my supervisor, Prof Nicholas M Spyrou, whose guidance and support is the key to my success in this long journey.

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I am deeply grateful to my brother Joseph and my sister Anita. Together they have been taking care of our aging mother, releasing me from my duty as the eldest son in the family. Without their effort, my path would have been much more difficult.

As you set out for Ithaka, hope your road is a long one, full of adventure, full of discovery. ... Ithaka gave you the marvellous journey. Without her you wouldn't have set out. She has nothing left to give you now. And if you find her poor, Ithaka won't have fooled you. Wise as you will have become, so full of experience, you'll have understood by then what these Ithakas mean. (Ithaka by Constantine Cavafy, 1863–1933)

Thank you Nicholas, πάρα πολύ.
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Chapter 1  Introduction

Cancer and radiotherapy

Worldwide, there are close to 11 million newly diagnosed cases of cancer per annum and approximately 6.7 million people dying of the disease in a year (IARC 2004). It is the number two killer after cardiovascular diseases according to the World Health Organisation (WHO 2002). It has been further estimated that about one-third of the population in the UK will be affected by some forms of cancer in their life and about one-quarter will die as a result (HMSO 1998, CRUK 2005). Over 270,000 new cases are diagnosed each year within the UK and more than 155,000 cancer patients die annually. Additionally, there are about 600,000 new cases of non-melanoma skin cancer (NMSC) every year. These cases are not included in the newly diagnosed statistics since NMSC is almost always curable. The top four most common cancers are breast, lung, large bowel and prostate cancers. Together they represent 53 % of all cases (Figure 1.1). They also constitute the top three cancers in each sex – prostate, lung and large bowel cancer in men; breast, large bowel and lung cancer in women (CRUK 2005).

Ten Most Common Cancer in the UK, 2001

![Diagram](image)

*Figure 1.1 Ten most common cancers in the UK in 2001 excluding NMSC (CRUK 2005)*
Cancer is clearly a burden to the health and the economics of a nation. It was estimated that cancer treatment has cost the NHS £1.3 billion every year (HMSO 1998). As early as 1992, the UK government had already identified cancer as one of five key areas to tackle for the health of the nation. Reduction targets were laid down for four types of largely preventable cancers: breast, cervical, skin and lung cancers (HMSO 1992). *The NHS Cancer Plan* (DoH 2000) is the first comprehensive plan for tackling the problem. It consolidates plans for prevention, diagnosis, treatment, care and research. Extra funding has been allocated and new machines, mostly medical linear accelerators (linac), have been procured for radiotherapy.

Surgery, radiotherapy and chemotherapy are the major treatment options for cancer (Figure 1.2). Each option has its own advantages and disadvantages. Their effectiveness depends on the type and the stage of the cancer. Oncologists frequently use a combination of these options to cure the disease.

![Major Cancer Treatment Options in the UK](image)

*Figure 1.2 Utilisation rate of major cancer treatment options in the UK. The rate includes all patients. However it is not clear how the data account for using a combination of treatment regimes, which is common practice by oncologists. (Data are compiled from RCR 2003)*

It is generally accepted that about 50–55% of all cancer patients benefit from radiotherapy treatments (ACIL 1998, RCR 2003). The survey by the Royal College of Radiologists (RCR 2003) shows that only 40% of the patients in the UK are treated with radiotherapy. This figure varies considerably in different regions mostly due to the availability of the facilities. Surveys in some other developed countries are showing similar figures except in Japan which is falling behind in this "league table" (Table 1.1). Teshima et al (1996) and Nakano (2004) cited that the patients and even
specialists were unaware of the benefits of radiotherapy as one of several reasons for their low utilisation rate.

<table>
<thead>
<tr>
<th>Country/Region</th>
<th>Radiotherapy utilisation rate</th>
<th>Reference</th>
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<tr>
<td>USA (overall average)</td>
<td>49 %</td>
<td>Teshima et al 1996</td>
</tr>
<tr>
<td>Victoria, Australia</td>
<td>42 %</td>
<td>ACIL 1998</td>
</tr>
<tr>
<td>Toronto, Canada</td>
<td>40 %</td>
<td>CCO 2004</td>
</tr>
<tr>
<td>Japan (overall average)</td>
<td>19 %</td>
<td>Teshima et al 1996</td>
</tr>
</tbody>
</table>

Table 1.1 Radiotherapy utilisation rate in some developed countries. The utilisation rate includes the newly diagnosed patients only.

Radiotherapy, or radiation therapy, is a class of techniques for treating diseases with ionisation radiation. The most commonly used radiations are high-energy photons and electrons whereas neutrons, protons and other heavy charged particles are still largely confined to research facilities. The radiation can be delivered to the tumour site using external radiation beams (teletherapy) or through surgical insertion of radioactive seeds directly into the tumour volume (brachytherapy). It is also possible to deliver the radiation through oral intake as in the treatment of thyroid cancer with iodine-131.

When radiation is delivered into a cell, it causes excitation and ionisation of the atoms along its path, which in turn cause a cascade of physical, chemical and biological changes. These changes cause cellular, enzyme and DNA damages. It has long been thought that DNA damage is the critical cause of cell death for there are about 1,000 single strand breaks and 40 double strand breaks per cell for every Gray of radiation (Steel 1996). Studies in the past decade suggest that damage to the signalling pathway within the irradiated cell may also cause cell deaths; damages to mitochondria or even to the cell membrane may trigger a cascade of events leading to cell death (Lewanski and Gullick 2001, Prise et al 2005). The bystander effect in which non-irradiated cells die together with the nearby, irradiated cells has also been observed (Prise et al 2005) but its relevance to radiotherapy is still uncertain (Mothersill et al 2004). Although irradiated, cells at different stages of the cell cycle
exhibit different radiosensitivities. Cells in mitosis or in the G₂ phase are the most sensitive to radiation damage whereas cells in the S phase are the least sensitive (Steel 1996). The actively growing tumour tissues are, therefore, more susceptible to radiation damage than the mature, less-active normal tissues. When the delivery of the radiation is carefully controlled, this difference in radiosensitivity allows the radiation to destroy the tumour cells and spare the surrounding normal tissues at the same time.

Radiation damage to normal tissues, especially near the field edge, might induce secondary cancers later on (Karlsson et al 1996, Epstein et al 1997). Mathematical modelling also suggests that different treatment plans have significant effect on the risk of radiotherapy-induced secondary cancer at distant sites from the original tumour (Lindsay et al 2001). These secondary cancers are caused by the scattered radiation; instead of killing the cells, it compromises the growth control mechanism primarily through a combination of radiation-induced mutations to the proto-oncogenes and to the tumour suppressor genes. Proto-oncogenes are normal genes whose activation through mutation will lead to excessive, uncontrolled cell growths. Tumour suppressor genes produce proteins (e.g., p53 protein from the TP53 gene) that, should the cell finds irreparable abnormalities at different checkpoints during the cell cycle, will lead to apoptosis – a pre-programmed self-destruction to prevent the cell from turning cancerous. The excessive expression of the proto-oncogenes and the dysfunction of the tumour suppressor genes may lead to cancer growth in general, not only from radiation. It was also argued that the radiation or other carcinogens may actually set up an environment, within the tissue, that encourages the natural selection of the carcinogenic cells (Breivik 2005). Thus, it is important to spare as much normal tissue as possible during a treatment course. Besides, there are organs at risk (OAR) and potential damage might cause severe harm to the patient or lead to a degraded quality of life. Sparing the OAR during treatment is the regime of three-dimensional conformal radiotherapy (3DCRT).

The goal of 3DCRT is to maximise the dose to the tumour while minimising the dose to the surrounding tissues. In other words, the three-dimensional distribution of the maximum dose conforms to the three-dimensional contour of the tumour. It is achieved by employing several radiation fields (beam portals) each of which is
shaped to the tumour’s cross-section presented to the beam. Although the maximum dose in each beam is not necessarily at the tumour site, the summed distribution has a maximum at the site.

In external beam radiotherapy, a linac is the most popular choice of delivery mechanism for its flexibility – most linacs today offer a choice of photon or electron beam and a choice of two or more energies, e.g. 6, 8, 10 and 25 MV, whereas the cobalt-60 machine offers a mean energy of 1.25 MeV. The higher energy beams have maximum dose deeper in the body, thus providing higher dose to a deep-seated tumour and better a skin sparing effect (Figure 1.3a). They also have a faster dose fall-off at the beam edge, that is, a more well defined beam (Figure 1.3b). Furthermore, a linac can deliver a high dose rate up to 10 Gy per minute as against 2 Gy per minute from a cobalt-60 machine. A higher dose rate translates to a shorter treatment time for the comfort of the patient and a higher patient throughput for the efficiency of the hospital.

![Percentage Depth Dose](image.png)

**Figure 1.3** Dose distribution in water phantom in 10×10 cm² field. (a) Percentage depth dose curves of three common megavoltage beams in a semi-infinite water phantom. The $d_{\text{max}}$ are 0.5, 1.5 and 3.2 cm for $^{60}$Co, 6 MV and 18 MV beams respectively. The curves are plotted from BIR (1996) data. (b) Isodose curves comparing cobalt-60 beam to a 4 MV beam (Johns and Cunningham 1983). It is clear that the higher energy beam has sharper beam edge. Note that the isodose curves of the $^{60}$Co beam are measured at 80 cm source-to-surface distance (SSD) whereas those of the 4 MV beam are at 100 cm SSD.
To shape the radiation field to the tumour’s outline, the multileaf collimator (MLC) is an essential component in the linac. A modern MLC consists of at least 40 pairs of independently controlled narrow leaves (Figure 1.4). They can be aligned closely to the cross-sectional contour of the tumour. The intensity modulated radiotherapy (IMRT) carries a step further than 3DCRT. Each MLC leaf moves to a different position at different time during the beam delivery creating a radiation field of varying fluence. The beam is thus shaped to the outline of the tumour and its fluence map conforms to the tumour’s 3D contour facing the beam. Although the machines are capable of delivering a shaped conformal beam, the accuracy of the dose calculation is of paramount importance to the success of a treatment; dose calculation is the starting point of a treatment plan and ultimately the treatment itself.

![Figure 1.4 The Elekta linac (Elekta 2005). (a) is the external view and (b) is its MLC consisting of 40 pairs of independent leaves each of which has a projected width of 1.1 cm at the centre of the isocentric plane.](image)

In 2002, there were 199 linacs and 8 cobalt-60 machines in the UK (NatCanSAT 2002, RCR 2003). Annually, the number of treatments per machine have been

---

1 Although the name IMRT suggests that the intensity is modulated, Webb (2001) argues that the name is a misnomer because the intensity is nearly a constant but the time integral of the intensity, i.e., the fluence, changes.
estimated at about 20,000 although there were only 102 treatment planning computers. Three quarters of these computers were over seven years old during the time these statistics were collected. Details of the machines and further breakdown of the figures can be found in NatCanSAT (2002). In view of these figures and the cancer statistics, it is not difficult for one to realise the high demand for fast, as well as accurate, treatment calculations.

**Dose calculations**

Currently, the method of choice for treatment planning calculation is the convolution superposition method for its efficiency. It is the heart and soul of the commercially available treatment planning systems, e.g., NOMOS CORVUS (Nizin 2001), CMS Focus (Miften et al 2000) and ADAC TPS (Huang et al 2002).

Figure 1.5 Dose kernels and the idea of superposition. (a) A point kernel is the spreading of dose from a point of interaction. (b) The superposition of point kernels is carried out at different depths as well as different positions in the radiation field. (c) A pencil kernel is the spreading of dose from a line of interactions. (d) The superposition of pencil kernels is carried out at different positions in the radiation field only. Dose at different depths is implicitly taken care of by the pencil kernel.
A dose deposition kernel from a pencil beam to a semi-infinite water phantom is pre-calculated, usually with Monte Carlo simulations (Figure 1.5a and c). The dose kernels from as many pencil beams as required to cover the whole radiation field are superimposed to give a 3D dose distribution (Figure 1.5b and d).

If the dose kernel is assumed to be spatially invariant, it is possible to speed up the calculation by convolving the kernel with the total energy released per unit mass, terma:

\[
D(\vec{r}) = \iiint T(\vec{r}') A(\vec{r} - \vec{r}') d^3\vec{r}'
\]  

where \( D(\vec{r}) \), \( T(\vec{r}) \) and \( A(\vec{r}) \) are the dose, the terma and the kernel value at point \( \vec{r} \) respectively. Terma can be calculated from the photon fluence, \( \Psi \), and the mass attenuation coefficient \( (\mu / \rho) \):

\[
T(\vec{r}) = \frac{\int_{E_{\text{min}}}^{E_{\text{max}}} (\mu(E)/\rho) \Psi(\vec{r}, E) E \, dE}{\int_{E_{\text{min}}}^{E_{\text{max}}} \Psi(\vec{r}, E) E \, dE}
\]  

Terma is usually chosen over the kinetic energy released per unit mass, kerma (e.g. Papanikolaou et al 1993, Liu et al 1997a, Ahnesjö and Aspradakis 1999), which is derived from the mass energy transfer coefficient \( (\mu_r / \rho) \):

\[
K(\vec{r}) = \frac{\int_{E_{\text{min}}}^{E_{\text{max}}} (\mu_r(E)/\rho) \Psi(\vec{r}, E) E \, dE}{\int_{E_{\text{min}}}^{E_{\text{max}}} \Psi(\vec{r}, E) E \, dE}
\]  

It is because \( (\mu / \rho) \) considers all the energy released by the photon at \( \vec{r} \) whereas \( (\mu_r / \rho) \) considers only the energy transferred to the site.

In any convolution or superposition calculation, heterogeneities in the body are accounted for, to some extent, by scaling the dose kernel according to electron densities in different tissues. Beam hardening, kernel tilting and body contour adjustments must also be considered. It is interesting to note that although the convolution superposition method is primarily an analytical calculation, the dose kernel is usually derived from a Monte Carlo calculation. A review on the convolution superposition method can be found in Ahnesjö and Aspradakis (1999).
Many studies (e.g. Huang et al 2002, Garcia-Vicente et al 2003, Jones and Das 2005) have shown that the convolution superposition method cannot fully account for the heterogeneities although the calculations are sufficiently accurate for most clinical applications. Roberts (2001) shows that a treatment planning calculation for a patient with metallic prosthesis has an error as high as 15% when compared to direct measurements and the error depends on the beam energy and the measurement depth in the body. At the same time, many authors have argued the case for Monte Carlo treatment planning (e.g. Andreo 1991, Bielajew 1994, Mohan 1997, Wang et al 1998, Ma et al 1999, 2000, DeMarco et al 2002a, Verhaegen and Seuntjens 2003) primarily because it is more compatible with experimental results, which is self-evident from Figure 1.6.

As the treatment regime moves from 3D-CRT to intensity modulated radiotherapy (IMRT), the complexity of the convolution superposition algorithm grows in an exponential manner and yet it still shows local discrepancy as large as 40% with respect to the Monte Carlo calculated dose (Verhaegen 2002). On the other hand, the Monte Carlo algorithm is essentially the same for 3D-CRT, IMRT, brachytherapy and a wide variety of radiation related calculations; there is no need to modify the Monte Carlo algorithm for dose calculations in simple or complex treatment regimes. More importantly, Laub et al (2000) and Ma et al (2000) show that the convolution
superposition calculations exhibit large discrepancies in the OARs. These discrepancies may affect the decision on the choice of treatment plans.

ICRU Report 50 and Report 62 (ICRU 1993, 2000) adopt the recommendation of +7,-5 % for dose heterogeneity, i.e., the dose at any point within the tumour should not exceed 107 % nor fall below 95 % of the prescribed dose. In fact, studies have shown that 5 % accuracy will have measurable impact on the treatment efficacy and ICRU Report 24 recommends this accuracy as an objective in dose delivery (ICRU 1976). The long-term goal has been subsequently revised to 2 % (ICRU 1987, Fraass et al 1998 and IAEA 2000a). ICRU Report 42 (ICRU 1987) specifically advises that the calculated dose should be within ±2 % of the measurement at the same point. All these requirements together constitute a demanding goal which is very difficult to achieve with the convolution superposition method. Accuracy is the primary motivation for the employment of the Monte Carlo method in treatment planning.

Monte Carlo calculation in treatment planning

The modern application of the Monte Carlo method in radiation transport problems is credited to Ulam and von Neumann in their work on neutron diffusion at the Los Alamos National Laboratory in the late 1940s (Metropolis 1987). Further developments in their neutron transport codes and the merging with photon and electron transport codes had eventually lead to the creation of MCNP, Monte Carlo N-Particle Transport Code System (Briesmeister 2000). By the late 1990s, the transport of proton and other particles were merged with MCNP and the codes were rewritten in Fortran 90 to form the MCNPX code (Waters 2002).

There is a wealth of papers validating and comparing the MCNP(X) codes with other transport codes in radiotherapy calculations (e.g. Chibani and Li 2002, Jeraj et al 1999, Love et al 1998, Reniers et al 2004, Schaart et al 2002, Siebers et al 1999). All these studies show that MCNP(X) is as suitable as any other code in radiotherapy calculations and MCNPX version 2.4.0 is the Monte Carlo code used in all the simulations in this thesis.
In essence, a Monte Carlo calculation is a virtual experiment, a theoretical experiment inside a computer: particles are generated, tracked through the geometry and finally escape or are absorbed. In the process, their interactions with different media in the geometry are accounted for and their contributions to the results or tallies are recorded. Furthermore, the tally will converge to a value because of the laws of large numbers. Its associated statistical error will conform to the central limit theorem. The solution thus obtained can, in principle, be arbitrarily accurate and precise. An immediate implication is that a Monte Carlo calculation will require an enormous computing resource because particles are tracked one by one and a large number of particles are probably needed such that rare but important events are not ignored. Typically, $10^7$ to $10^8$ source particles are needed.

The accuracy of a Monte Carlo calculation depends on how the underlying physics is represented in the models and in the cross section data, the Monte Carlo algorithm sampling of the cross section data and the method of accumulating the results. The precision depends, to a large extent, on the number of particles tracked or simulated.

One way to speed up the computation is to employ a faster computer, which is costly, or to use parallel processing with a cluster of inexpensive computers. The Monte Carlo method is intrinsically parallelisable. The initial source particles are independent from each other. They can be tracked independently on separate machines and the results are combined at the end. Without dwelling on the more sophisticated parallelising schemes, it suffices to say that more processors will provide faster computation speed. Although the cost of hardware decreases over time, it is not always possible to increase the number of processors for faster calculations or for more complex calculations. A software solution is always a welcome complementary to the hardware solutions.

Monte Carlo calculations are often divided into several steps so that some of the calculations need not to be repeated. In the simulation of a linac, the patient independent components can be simulated once and the emerging particles are recorded in a phase space file. This file will be the source for subsequent simulations of the patient specific components. Additionally, certain variance reduction techniques (VRTs) can be applied when the simulation is carried out in steps.
As mentioned before, a Monte Carlo simulation tracks several millions of particles. The phase space file from the patient independent components typically requires gigabytes of storage. It is inconvenient for routine manipulations. This thesis proposes a novel technique, termed the directional spectrum approach, for the examination of the phase space data. The technique is totally data driven as there is no pre-conceived model for the data to fit in. The information of the phase space is visualised and analysed with different data plotting methods. An end result is that these graphs will suggest a model which will accurately summarise the information. This compact model is termed the directional spectrum model (DSM). The DSM couples the particle's energy spectrum to its position on the phase space plane and its direction vector whereas other established models loosely relate the energy spectrum to the particle origin, especially to its direction vector. This is where the DSM distinguishes itself from all other models.

In summary, Monte Carlo treatment planning is coming of age. It provides an accurate way to calculate a radiotherapy treatment plan. At the very starting point of the calculation, there is a phase space model that describes the radiation beam generated by the linear accelerator. A successful model is therefore absolutely essential in the combat against the number two killer, cancer, of the world. This thesis is a study of the Monte Carlo method and the phase space model.

**Thesis outline**

Chapter 2 is a review of the physics commonly encountered in radiotherapy and the Monte Carlo modelling of such physics. Some variance reduction techniques will be discussed. The errors associated with the interaction cross sections will also be addressed.

Chapter 3 describes the basic principles of the linear accelerator with particular focus on the geometry of Elekta SLi treatment head. The details of its Monte Carlo simulation, including the generation of the phase space file with MCNPX, will be discussed.
Chapter 4 reviews the existing phase space models. Two models are implemented and their relative merits are discussed.

Chapter 5 describes the directional spectrum approach to analysing the phase space data and how this data-driven approach leads to the development of the directional spectrum model (DSM) of the phase space.

Chapter 6 explores the use of the DSM in IMRT applications, in particular, the fields shaped by the MLC. The beam penumbras and the shifts in isodose curves will be examined. Denoising techniques will also be discussed.

Chapter 7 is the conclusion and a discussion on possible future work.
Chapter 2  The Monte Carlo Method

Using the Monte Carlo method to solve a difficult problem is nothing new. A famous one is the calculation of $\pi$ by dropping a needle of length $l$ randomly onto a parallel grid of width $d$ in Buffon's needle problem in which the probability $p$ of the needle touching or crossing a grid line is $p = 2l/\pi d$. By experimenting with a needle and a grid of known dimensions, the probability $p$ can be approximated and therefore $\pi$ can be estimated. In the case of radiation transport, it is possible to formulate the transport with the Boltzmann transport equation which is an integral-differential equation. However, the success of solving the equation analytically is limited to relatively simple geometries (Boman 2005). The Monte Carlo method is another way to solve a transport problem regardless of the complexity of the geometry.

Random walk and sampling

The Monte Carlo method is a random walk: each decision is made by sampling a relevant probability distribution with a random number. To illustrate the use of a random number, consider the distance a photon will travel before its next interaction in a medium. The probability $p(l)dl$ of a photon travelling a distance $l$ and interacting with the medium at a point between $l$ and $l + dl$ is the probability of the photon travelling a distance $l$ without interaction multiplied by the probability of it interacting immediately afterwards (within a distance $dl$):

$$p(l)dl = e^{-\mu l} \mu dl \quad \text{(2.1)}$$

where $\mu$ is the linear attenuation coefficient associated with the energy of the photon. Since $p(l)dl$ describes the probability of photon interactions, $p(l)$ is called the probability density function. Then, $P(l)$, the integral of $p(l)$, is the cumulative distribution function (CDF):
The Monte Carlo Method

\[ P(l) = \int_0^l p(s) ds = 1 - e^{-\mu l} \quad \ldots \quad 2.2 \]

It can be proved that \( P(l) \) is uniformly distributed in the interval \([0,1)\). Let \( \xi \) be a uniformly distributed random number in \([0,1)\) and

\[ \xi = P(l) = 1 - e^{-\mu l} \quad \ldots \quad 2.3 \]

\[ l = -\frac{1}{\mu} \ln(1 - \xi) \quad \ldots \quad 2.4 \]

Since \( \xi \) is uniformly distributed in \([0,1)\), so is \( (1 - \xi) \) and thus, \( l \) can be expressed as

\[ l = -\frac{1}{\mu} \ln(\xi) \quad \ldots \quad 2.5 \]

That is, we can randomly generate \( \xi \) in \([0,1)\) and use Equation 2.5 to predict how far the photon will travel before its next interaction. This method of sampling is known as the inversion of the cumulative distribution function (CDF). After an interaction is known to occur, we can then determine the type of interaction and the outcome of the interaction using similar method of sampling the inverse of the CDF or using other sampling techniques, provided that further cross section data for different interactions are available.

**Random number generator**

It is not difficult to conceive how one can generate a sequence of truly random numbers. For example, a random number can be obtained from the time interval between the detection of two consecutive radioactive decays. Unfortunately, a sequence of such random numbers cannot be reproduced and is thus useless in many circumstances – debugging the Monte Carlo code would be impossible and repeating a virtual experiment would also be impossible. A useful sequence of random numbers must be reproducible and apparently random. It is not truly random. It is *pseudorandom*. In the following discussion, random number will assume the meaning of pseudorandom number.
The Monte Carlo Method

A very reliable, robust (pseudo-) random number generator comes from the linear congruential method, LCG\((a, c, m)\):

\[
s_{n+1} = (as_{n} + c) \mod m
\]

... 2.6

where \(s_{n}\) and \(s_{n+1}\) are the \(n^{th}\) and the \(n+1^{st}\) integer random numbers (\(s_{0}\) is also known as the seed) for some predetermined positive integers \(a, c\) and \(m\). A random number \(\xi_{i}\) in the interval \([0,1)\) is then obtained from

\[
\xi_{i} = s_{i} / m
\]

... 2.7

The sequence of random numbers generated by the LCG method depends entirely on the values of \(a, c\) and \(m\). A treatment on their choices can be found in Knuth (1998). A suitable combination of \(a\) and \(m\) is of paramount importance. Inappropriate values will lead to an ill-behaving random number sequence – non-randomness and correlation among the numbers. A wrong choice of \(a\) may even lead to a useless sequence of zeros (Briesmeister 2000). The choice for \(c\) is not very critical although certain values may result in a less-than-maximum period. It is obvious from Equation 2.6 that the maximum period of the random number sequence is \(m\). Skipping a fixed number of random numbers may also increase the apparent randomness of the sequence (Knuth 1998) although this view is not shared by James (1990).

A common choice for \(m\) is \(2^{b}\) where \(b\) is the word size of the computer running the generator so as to maximise the period without special mathematical routines. For example, a 32-bit computer can provide in principle over 4 billion random numbers under this scheme before the sequence is repeated. The actual period is also determined by the choice of \(a\) and \(c\) (Knuth 1998).

The LCG in MCNP has a period of \(2^{46} \approx 7.04 \times 10^{13}\) random numbers. The default values for \(a\) and \(s_{0}\) are \(5^{19}\) and \((5^{19})^{152917}\) respectively. Also by default, MCNP assumes that 152917 random numbers are sufficient for a history. The starting random number for a new history is 152917 positions up the sequence from the starting random number of the last history. This skipping of random numbers is called the random number stride. It increases the randomness of the generated random numbers. MCNP allows users to modify these default values via the DBCN.
card in the input file. In view of Knuth's (1998) analysis, the random number seed and the stride, but not the multiplier $a$, may be modified without affecting the quality of a simulation.

**Photon transport**

Photon interaction with matter is relatively infrequent. A 1 MeV photon is expected to travel, on average, about 10 cm (mean free path) in water before any interaction. As mentioned previously, the distance to the next interaction can be calculated from the linear attenuation coefficient (Equation 2.5). The type of interaction is then sampled from the linear coefficients of individual reactions. For the photon energies in most medical applications, the reactions are photoelectric absorption, Compton scattering, Rayleigh scattering, pair production and photonuclear reactions with cross sections $\sigma_{pe}$, $\sigma_{incoh}$, $\sigma_{coh}$, $\sigma_{pp}$ and $\sigma_{pn}$ respectively. The total cross section $\sigma$ is the sum of individual reaction cross sections.

$$\sigma = \sigma_{pe} + \sigma_{incoh} + \sigma_{coh} + \sigma_{pp} + \sigma_{pn} \quad ... \ 2.8$$

Sampling for the reaction type is straightforward. Given that a reaction has occurred, the probability $p_i$ of that $i$ is the reaction is:

$$p_i = \frac{\sigma_i}{\sigma} \quad ... \ 2.9$$

$$\sum_i p_i = 1 \quad ... \ 2.10$$

Then, a CDF can be constructed and sampled with the inversion method.

Webb and Parker (1978) considered a simplified situation in which only photoelectric absorption, Compton scattering and pair production are present in water. The relative probabilities of each interaction are:

$$p_{incoh} = \frac{\sigma_{incoh}}{\sigma} ; \quad p_{pe} = \frac{\sigma_{pe}}{\sigma} ; \quad p_{pp} = \frac{\sigma_{pp}}{\sigma} ; \quad \sigma = \sigma_{pe} + \sigma_{incoh} + \sigma_{pp} \quad ... \ 2.11$$

For a random number $\xi$, the collision type is determined by:
The Monte Carlo Method

If \( \xi - P_{PE} \leq 0 \) then it is photoelectric absorption;
if \( \xi - P_{PE} > 0 \) and \( \xi - P_{PE} - P_{Incoh} \leq 0 \) then it is Compton scattering;
if \( \xi - P_{PE} - P_{Incoh} > 0 \) then it is pair production.

This method is actually equivalent to a sequential search through the cumulative probability table. Since Compton scattering is the dominant interaction in water in the energy range of interest to medical physics, the above arrangement usually requires two comparisons to determine an interaction type. If the authors had considered Compton scattering before photoelectric absorption, the search would have required only one comparison most of the time. Also, the sampling efficiency would have been significantly affected should more interaction types be included. The binary search of the CDF table is more general and efficient.

The above description applies to a medium of single element. When the medium is a mixture instead of a pure element, the Mixture Rule for the mass attenuation coefficient applies. The total cross section \( \sigma \) is related to the linear attenuation coefficient \( \mu \) through the following equation

\[
\mu = \sigma \rho \frac{N_A}{A_w} \quad \text{... 2.12}
\]

or equivalently in terms of mass attenuation coefficient,

\[
\left( \frac{\mu}{\rho} \right) = \sigma \frac{N_A}{A_w} \quad \text{... 2.13}
\]

where \( \rho \), \( N_A \) and \( A_w \) are the mass density, Avogadro’s number and the atomic weight of the element. The Mixture Rule states that the mass attenuation coefficient \( (\mu/\rho)_M \) is the weighted sum of the mass attenuation coefficients of constituent elements \( (\mu/\rho)_i \):

\[
(\mu/\rho)_M = \sum_i (\mu/\rho)_i w_i \quad \text{... 2.14}
\]

such that \( w_i = m_i / \Sigma m_i \) is the element’s proportion by mass in the mixture. The Mixture Rule is inapplicable to energies near the absorption edges of compounds where the molecular binding affects the binding energy of the electrons.
Figure 2.1 shows the photon interaction cross sections important in most medical physics applications. The most abundant elements in the human body are hydrogen, carbon, nitrogen, oxygen, and calcium with atomic numbers below 20. The photon energies of interest are usually below 25 MeV, e.g., $^{192}\text{Ir}$ photon emission is between 61.5 keV and 1.3 MeV while some modern linear accelerators have bremsstrahlung photon energies up to 25 MV. Even in high-Z elements like lead and tungsten used as targets in the generation of bremsstrahlung photons and in shielding materials, the Compton effect is still very important.

![Figure 2.1 Dominant interactions with respect to photon energy and the atomic number of the medium (modified from Evans 1955). $\tau$, $\sigma$ and $\kappa$ are the cross sections of the photoelectric effect, Compton effect and the pair production respectively. For most medical physics interactions in the human body (shaded area), Compton effect is the main interaction type.](image)

**Photoelectric reaction**

![Figure 2.2 Photoelectric absorption.](image)

In the event of photoelectric absorption, the incident photon interacts with an atomic electron (Figure 2.2). The photon is absorbed and the electron is emitted from the
atom. The photoelectron will have energy $T = h\nu_0 - B$ where $h\nu_0$ is the incident photon energy and $B$ is the binding energy of the electron. Since photoelectric absorption occurs predominantly with the K electron, most codes assume that this reaction in the K shell is the only reaction and all the available energy is transferred to the photoelectron. The emission angle (polar angle, $\varphi$, Figure 2.3) is nearly 90° at low incident photon energy. As the incident energy increases, the polar angle decreases.

Webb and Parker (1978) suggest using the low energy relationship to sample for the polar angle $\varphi$:

$$\frac{dN}{d\varphi} \propto \sin^3 \varphi$$  \hspace{1cm} ... 2.15

Thus,

$$\xi_1 = \frac{3}{4} \int_0^\varphi \sin^3 \phi \, d\phi$$  \hspace{1cm} ... 2.16

and solve for $\varphi$. The azimuthal angle $\theta$ is sampled uniformly in $[-\pi, \pi)$:

$$\theta = \pi(2\xi_2 - 1)$$  \hspace{1cm} ... 2.17

Figure 2.3 Definition of polar angle and azimuthal angle. Note that the angles are relative to the incidence direction. Subsequent tracking of the scattered/emitted particle requires a translation of this frame of reference to the laboratory frame of reference.
After the electron is ejected, there will be a cascade of characteristic x-rays or Auger electrons. These secondary particles are assumed to be emitted isotropically and shall be banked for subsequent tracking. The photoelectron will then be tracked. The electron transport is very different from photon transport because of its frequent interaction with the medium through the Coulomb force. The generation of characteristic x-rays and Auger electrons will be discussed later with the electron tracking algorithms.

Materials of atomic number Z below 12 have fluorescence photons or characteristic x-rays with energy less than 1 keV. They are assumed to be re-absorbed immediately by most general purpose Monte Carlo codes. For example, a 1 keV photon has mean free path less than 0.001 cm in water. A photoelectric event in such cases is often considered a terminal event with all of its energy deposited locally.

**Compton scattering**

The energies and flight directions of the scattered photon and the recoil electron after a Compton event (Figure 2.4) are determined by the Klein-Nishina cross section:

\[
\frac{d\sigma_{KN}}{d\Omega} = \frac{r_0^2}{2} \left( 1 + \cos^2 \varphi \right) \left( \frac{1}{1 + \alpha (1 - \cos \varphi)} \right)^2 \left( 1 + \frac{\alpha^2 (1 - \cos \varphi)^2}{[1 + \alpha (1 - \cos \varphi)][1 + \cos^2 \varphi]} \right)
\]

... (2.18)

where

\[
r_0 = \frac{e^2}{m_0 c^2}.
\]

... (2.19)

\[
\alpha = \frac{\hbar \nu_0}{m_0 c^2}.
\]

... (2.20)

\(e\) is the electron charge, \(m_0\) the electron rest mass, \(\hbar \nu_0\) the initial photon energy and \(\varphi\) the polar angle of the scattered photon.

Sampling the Klein-Nishina cross section for the polar angle \(\varphi\) is far from trivial. Some authors attempted by fitting an equation to the cross section data and it was claimed that the accuracy was within 1 % (Webb and Parker 1978). Alternatively, it can be sampled with the acceptance-rejection technique. MCNP uses methods
developed by H. Khan for energies below 1.5 MeV and by L. Koblinger for energies above 1.5 MeV and these methods sample the Klein-Nishina cross section exactly (Briesmeister 2000).

\[
\begin{align*}
    p_0 &= p \cos \varphi + p' \cos \varphi' \\
    p \sin \varphi &= p' \sin \varphi' \\
    h\nu_0 &= h\nu + T \\
    p'c &= \sqrt{T(T + 2m_c^2)}
\end{align*}
\]

Solving the equations, the scattered photon energy \( h\nu \) is

\[
h\nu = \frac{h\nu_0}{1 + \alpha(1 - \cos \varphi)}
\]

The recoil electron has kinetic energy \( T \)

\[
T = h\nu_0 \frac{\alpha(1 - \cos \varphi)}{1 + \alpha(1 - \cos \varphi)}
\]

and polar angle \( \varphi' \) of initial flight direction.
The azimuthal angles for both the scattered photon and the recoil electron are sampled uniformly in \([-\pi, \pi]\) (Figure 2.3).

Strictly speaking, the Klein-Nishina cross section is derived for the interaction with a free electron at rest. To account for the binding effect, the probability of an electron leaving the atom at an angle \(\varphi\) is approximated by the Klein-Nishina probability which gives the electron a momentum \(p'\) multiplied by the probability of the electron with this momentum actually leaving the atom (Equations 2.28 and 2.29). This second probability is called the incoherent scattering function \(S(x, Z)\) where \(x\) is a function of the momentum transferred to the recoil electron and \(Z\) is the atomic number of the element (Hubbell et al 1975). The Compton differential cross section and total cross section for a single electron are given by

\[
\frac{d\sigma_{\text{incoh}}}{d\Omega} = \frac{d\sigma_{\text{KN}}}{d\Omega} S(x, Z) \quad ... 2.28
\]

\[
e^{\gamma \sigma_{\text{incoh}}} = \left( \int_0^{2\pi} \frac{d\sigma_{\text{KN}}}{d\varphi} \right) S(x, Z) 2\pi \sin \varphi \, d\varphi \quad ... 2.29
\]

and the Compton cross section for an atom is

\[
\sigma_{\text{incoh}} = e^{\sigma_{\text{incoh}} \cdot Z} \quad ... 2.30
\]

Since the electron in orbit is not at rest, the energy of the incident photon seen by the electron differs from the true energy due to Doppler effect. Some Monte Carlo codes (e.g. MCNP5 and MCNPX 2.5) can sample the Doppler broadened spectrum for the incident photon energy to account for the motion of the electron (McKinney et al 2005).

**Rayleigh scattering**

Rayleigh scattering is sometimes ignored because the incident photon does not lose energy and its flight direction changes very little (Figure 2.5). In fact, MCNP offers Rayleigh scattering as an option. Its consideration can be turned on or off as desired.
The Monte Carlo Method

The Rayleigh differential cross section \( \frac{d\sigma_{coh}}{d\Omega} \) is the Thomson scattering cross section \( \frac{d\sigma}{d\Omega} \) multiplied by a form factor:

\[
\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2} \left(1 + \cos^2 \varphi \right) \quad \text{... 2.31}
\]

\[
\frac{d\sigma_{coh}}{d\Omega} = \frac{r_0^2}{2} \left(1 + \cos^2 \varphi \right)[F(x, Z)]^2 \quad \text{... 2.32}
\]

\[
\sigma_{coh} = \frac{2\pi r_0^2}{2} \left(1 + \cos^2 \varphi \right)[F(x, Z)]^2 2\pi \sin \varphi \, d\varphi \quad \text{... 2.33}
\]

where \( r_0 = \frac{e^2/m_e c^2}{2} \) is the electron radius and \( F(x, Z) \) is the form factor by Hubbell et al (1975). To sample for \( \varphi \), we can use the technique in Compton scattering: sample the Thompson cross section, i.e., without the form factor, and use the form factor to adjust the probability of whether the photon is scattered. The azimuthal angle \( \theta \) is again sampled uniformly in a manner similar to that of a Compton scattered photon (Figure 2.3).

![Rayleigh scattering](image)

**Figure 2.5 Rayleigh scattering.**

**Pair production**

In the event of pair production, the photon is absorbed by the electric field of the nucleus. A pair of electron and positron are emitted (Figure 2.6). The differential cross section is given by (Bethe and Heitler 1934, Heitler 1954):

\[
\frac{d\sigma_{pp}}{d\Omega} = \frac{Z^2}{137} \frac{r_0^2}{2\pi} \left(\frac{m_e c^2}{2\pi} \right)^2 F_{pp} \quad \text{... 2.34}
\]

where \( F_{pp} \) is a complicated function of momentum, energy and angle projection. The cross section includes the triplet production in which an atomic electron is ejected.
The Monte Carlo Method
together with the electron-positron pair produced. The triplet production has a relatively small probability, in the order of $1/Z$ of the pair production. Hence, triplet is actually important in low-Z materials like water and tissue. However, it is not modelled explicitly by many Monte Carlo codes but its cross section is incorporated into the pair production cross section.

![Figure 2.6 Pair production.](image)

Webb and Parker (1978) gave the following approximation to the pair production:

$$\varphi = 1/\hbar \nu_0$$

where $\varphi$ is the polar angle of the emitted electron and positron and they assumed that the electron and the positron share the kinetic energy equally, i.e., $T_+ = T_-$. The azimuthal angle $\theta$ is again sampled uniformly in $[-\pi, \pi)$ (Figure 2.3). If $(u,v,w)$ is the direction vector of the electron such that

$$u = \cos \phi; \quad v = \sin \phi \cos \varphi; \quad w = \sin \phi \sin \varphi; \quad \|u, v, w\| = 1$$

then the positron’s direction is simply $(u, -v, -w)$.

Figure 2.7 shows two plots of the electron energy distributions from pair production. A quick examination of the figure clearly negates the equal energy sharing assumption made by Webb and Parker (1978). At high energies (above 20 MeV), each curve has a broad minimum around 0.5 where electron and positron share the photon energy equally. It means that equal sharing of the photon energy between the electron and the positron is not the most likely outcome. At lower energies, each curve has a broad maximum centred at 0.5. This means that many different
combinations of energy sharing are almost as likely as a 50-50 sharing. In fact, the
curve at 1.5 MeV is nearly flat in the whole range of energies! Furthermore, the
positron experiences a repulsive force from the nucleus and the electron experiences
an attractive force. The positron should have slightly more kinetic energy than the
electron. An exact calculation should show the curves slightly skewed to the right
hand side. The symmetry comes from Born’s plane wave approximation. Because of
conservation of momentum, the polar angles of the electron and the positron should
be calculated from their energies.

![Figure 2.7 Pair production probability as a function of the positron kinetic energy (Bethe and Heitler 1934). The positron kinetic energy \( E_+ \) is expressed in terms of a fraction of the incidence photon energy transferred to the positron and the electron. The cross section \( \Phi \gamma \) is expressed in the unit of \( (Zr^2)^{1/37} \). Each curve represents an incidence photon energy as multiples of the electron rest mass. Thus the curve in (a) from the bottom are 1.5 MeV, 3 MeV and 5 MeV; the curves in (b) are 5 MeV, 10 MeV, 25 MeV, 50 MeV, 500 MeV and an asymptotic solution for energy approaching infinity.](image)

A justification for the equal-energy sharing scheme is that both the electron and the
positron lose energy quickly in a medium through collisions and bremsstrahlung
production. Also, the tortuous electron/positron path in the medium will “wash out”
the effect of the initial polar angles (flight directions) quickly.

**Photonuclear reactions**

The average binding energy per nucleon in the nucleus is about 8 MeV. When the
nucleus absorbs a photon with incidence energy above its nucleon binding energy,
the nucleus is excited to a higher energy state. Subsequent de-excitation may emit
one or more nucleons. This process is known as photonuclear disintegration – \((\gamma, x)\)
reactions, where x stands for particle or particles emitted from the nucleus. In the energy range (below 25 MeV) of most medical applications, single neutron emission – the (γ, n) reaction – is the main reaction channel among all photonuclear events. These photoneutrons are generated in the giant dipole resonance (GDR) region of about 5 MeV to 30 MeV. The neutron emission is assumed to be isotropic.

**Photon cross section data**

A discussion on how the cross section data were derived is beyond the scope of this work. Some of the data came from measurements while others were derived theoretically. In summary (Storm and Israel 1970), the Compton cross section is derived from the numerical integration of the Klein-Nishina differential cross section and the incoherent scattering function is derived from wave functions; the Rayleigh cross section comes from the Thomson cross section and the wave-function derived form factor; the pair production cross section is derived from quantum mechanics; the photoelectric cross section comes from the measured total cross section subtracted by the other cross sections.

<table>
<thead>
<tr>
<th>Photon cross section</th>
<th>Estimated accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>photoelectric</td>
<td></td>
</tr>
<tr>
<td>1–6 keV</td>
<td>10 %</td>
</tr>
<tr>
<td>6–200 keV</td>
<td>3 %</td>
</tr>
<tr>
<td>&gt; 200 keV</td>
<td>10 %</td>
</tr>
<tr>
<td>Compton</td>
<td></td>
</tr>
<tr>
<td>total</td>
<td>3 %</td>
</tr>
<tr>
<td>absorption</td>
<td>10 %</td>
</tr>
<tr>
<td>scattering (total – absorption)</td>
<td>10 %</td>
</tr>
<tr>
<td>Rayleigh scattering</td>
<td>3 %</td>
</tr>
<tr>
<td>Pair production</td>
<td>5 %</td>
</tr>
<tr>
<td>Total cross section</td>
<td>5–10 %</td>
</tr>
</tbody>
</table>

*Table 2.1 Photon cross section accuracy given by Storm and Israel (1970). The total cross section error depends on which interaction is dominant. In the photoelectric dominant and the pair production dominant regions, the error is as much as 10%. In the Compton region, the error is about 5%.*
The older version of MCNP photon library, mcplib, uses the data from Storm and Israel (1970). The dataset includes elements from \( Z = 1 \) to \( Z = 100 \) and for energies from 1 keV to 100 MeV. The authors estimated the accuracy of their data to be within the range of 3 % to 10 % (Table 2.1).

Hubbell (1997) reviewed the use of the incoherent scattering function \( S(x,Z) \). He concluded that \( S(x,Z) \) has less than 5 % error for small angles but it could be as much as 20 % for large angles and in high-Z materials. This conclusion has significant implication on all photon cross section data because \( S(x,Z) \) is used in the calculations of both the Compton cross section and the pair production cross section. Also, a related function \( F(x,Z) \) is used in the Rayleigh cross section.

Chantler (1995, 2000) also reviewed the form factors and the photoelectric cross sections near the absorption edges for energies between 1 eV and 1 MeV. The errors were accumulated from the minor errors of the electronic wave function distributions, particularly near the edges, in the inner orbits. Thus, the values near the K edges are more accurate than the other edges. Within 10 % of the K edge, the estimated errors were 10 % in monatomic gases and 10–20 % in condensed phases. Within 0.1 % of the other edges, they were 20–30 % and 50 % in monatomic gases and in condensed states respectively.

It is well known that the mcplib data is giving erroneous results in low-energy, 10–150 keV, photon simulations (DeMarco et al 2002b, Ye et al 2004). The current versions of MCNP come with more up-to-date libraries mcplib02, mcplib04 based on EPDL (Cullen et al 1989, Cullen et al 1997) and the results are more consistent with other Monte Carlo codes.

Boone and Chavez (1996) compared the Storm and Israel (1970) data and their computer program MUCOEFF. MUCOEFF is also based on EPDL89 like mcplib02. The authors found that the two sets of data are generally within 5 % of each other. However, the K- and L-edge energies are not exactly the same in the data sets. Some elements therefore exhibit a large discrepancy (Figure 2.8 and Figure 2.9).
Hughes (1993) compared the two MCNP photon libraries *mcplib* and *mcplib02*. In contrast to Boone and Chavez (1996), the author found the maximum fractional differences are 0.01 % for the coherent cross section, 0.786 % for the incoherent cross section, 0.0721 % for the photoelectric cross section, and 4.37 % for the pair plus triplet cross section. The fractional difference was defined as the difference in the cross sections divided by the total cross section in *mcplib02*.

Cullen *et al* (1997) estimated the error of photoelectric cross section in the EPDL97 database to be 1–2 % in the range of 5 keV to 10 MeV. This is far better than the Storm and Israel (1970) data of 3–10 %.
Many other photon cross section data sets have also been published over the years, for example, Hubbell et al (1980), Plechaty et al (1981), Henke et al (1982), Hubbell (1982), Hubbell and Seltzer (2004), etc. XCOM by Berger et al (1998) at the National Institute of Standards and Technologies is a computer program for generating the photon cross section data. Hubbell (2000) recommended the use of this library. For an extensive review of cross section data relevant to medical physics application, one may refer to Hubbell (1999, 2000).

One implication from the relatively large error in the photoelectric cross section is that the low energy cut-off should be set at a “reasonable” level. Transporting all low-energy photons does not help increasing the simulation accuracy. It is likely to decrease the accuracy because of the large error in the cross section. Whenever local deposition of the photon energy can be assumed, the cut-off should be set to reflect that. An added benefit is the increase in computing efficiency because unnecessary particles are not tracked.

The photonuclear cross section is generally not included in the photon cross section database, but published separately (IAEA 2000b). It contributes about 5% to the total cross section at the peak of the resonance (Hubbell 1999).

**Electron transport**

Unlike photons, electrons interact almost continuously with the medium because of the long range of the Coulomb force. The photon mean free path $\bar{l} = 1/\mu$ is about 10 to 1000 times the electron continuous slow-down approximation (CSDA) range in water in the medical application energy range (Figure 2.10).
The Monte Carlo Method

The CSDA range of electron $R_0$ is the distance an electron will travel before losing all of its kinetic energy entirely through soft interactions, i.e., energy loss at each interaction is small compared to the initial energy (ICRU 1984).

\[ R_0 = \int_0^{T_0} \frac{dT}{S_{\text{tot}}(T)} \]  \hspace{1cm} \text{(2.37)}

where $T_0$ is the initial electron energy and $S_{\text{tot}}(T)$ is the total stopping power of electron in the medium defined as the amount of energy loss by the electron per unit path length.

It was estimated that an electron undergoes about $10^4$ times more interactions with the medium than a photon of the same energy (Grosswendt 1996). Tracking all electron interactions is clearly unrealistic with our current computer hardware technology. Berger (1963) pioneered the condensed history method for electron transport (Figure 2.11). There are two major strategies known as Class I and Class II electron transports. Class I electron transport assumes that, for a predetermined small energy loss, the electron will travel a fixed distance and its angular deflection can be approximated analytically. Knock-on ($\delta$) electrons and bremsstrahlung photons are produced at the end of each step. Class II electron transport simulates individual "hard events" and the track between two hard events is treated with the continuous
slow-down approximation. A hard event is a collision involving energy exchange above a predetermined threshold.

![Figure 2.11 Realistic and simulated electron tracks. A realistic electron track (a) has many interactions, too many for a practical analog simulation. A practical simulation (b) uses the condensed history technique in which only some events are simulated while the rest are approximated by various theories. The area between thick lines represents the electron track bundled with the electron “discourse” due to multiple scatterings. This drawing is a Class II electron transport.](image)

**Electron and positron stopping powers**

ICRU Report 37 (ICRU 1984) reviewed the electron and positron stopping power calculations and related cross section data. Stopping power is the average energy loss by a charged particle per unit path length. The total stopping power $S_{\text{tot}}(T)$ is the sum of the collision stopping power $S_{\text{col}}(T)$ due to ionisation and excitation and the radiative stopping power $S_{\text{rad}}(T)$ due to bremsstrahlung production.

$$S_{\text{tot}}(T) = S_{\text{col}}(T) + S_{\text{rad}}(T)$$  \hspace{1cm} (2.38)

In contrast to the radiative stopping power in which energy is carried far away from the electron track, the collision stopping power involves energy deposition relatively close to the track. However, this is not the same as the concept of energy deposited “locally.” This is because the knock-on electrons or the $\delta$-rays may travel a substantial distance in the medium. For energy to be considered deposited locally, these secondary electrons must lose all of their kinetic energy in a short distance from the primary track. This means that the secondary electron is allowed to have very small energy or alternatively, the energy exchange is below a certain energy
threshold. This leads to the definition of restricted collision stopping power $L_{\Delta}(T)$. It is the average energy loss per unit path length due to collisions involving energy exchange below a predetermined energy threshold $\Delta$. The concept of restricted stopping power is very useful in Monte Carlo calculations, especially in Class II electron transports.

ICRU Report 37 quoted the following estimated errors in stopping powers:

<table>
<thead>
<tr>
<th>Energy</th>
<th>Estimated error in $S_{\text{col}}(T)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$&lt;10$ keV</td>
<td>10-15%</td>
</tr>
<tr>
<td>10-100 keV</td>
<td>2-3% (low Z)</td>
</tr>
<tr>
<td>$&gt;100$ keV</td>
<td>1-2%</td>
</tr>
</tbody>
</table>

*Table 2.2 – Estimated error in collision stopping power for electrons/positrons (ICRU 1984).*

<table>
<thead>
<tr>
<th>Energy</th>
<th>Estimated error in $S_{\text{rad}}(T)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$&lt;2$ MeV</td>
<td>5%</td>
</tr>
<tr>
<td>2-50 MeV</td>
<td>2-5%</td>
</tr>
<tr>
<td>$&gt;50$ MeV</td>
<td>2%</td>
</tr>
</tbody>
</table>

*Table 2.3 – Estimated error in radiative stopping power for electrons/positrons (ICRU 1984).*

Analogous to the Mixture Rule in photon mass attenuation coefficients, there is an additive rule for the mass collision stopping powers:

$$(S_{\text{col}} / \rho) = \sum w_i (S_{\text{col}} / \rho)_i$$

... 2.39

where $w_i$ and $(S_{\text{col}} / \rho)_i$ are the proportion by mass and the collision stopping power of element $i$ in the mixture. Since the density of the medium is a very important factor in the stopping power, there is a density correction factor in the stopping power calculations. The additive rule does not correctly predict this density correction factor for the mixture.
Also involved in the stopping power is the mean excitation energy. Each element has different values for gas and for condensed phases; it is also different when molecular binding is taken into account. The additive rule for stopping powers is not as satisfactory as the Mixture Rule for photon attenuation coefficients, which breaks down only near the absorption edges. Sternheimer (1981) investigated the formulation of the density correction factor which is described in detail by Nelson et al (1985).

The difference between electron stopping power and positron stopping power is small but noticeable (Figure 2.12). MCNP treats a positron the same as an electron except that the positron will annihilate with a stationary electron at the end of its track. Other codes, e.g. EGS4, treat them separately.

\[
\sigma_{2\gamma} = 4\pi r_0^2 \frac{c}{v} \quad \text{for } v \ll c
\]

where \( c \) and \( v \) are the speed of light and the speed of the positron. Thus the annihilation cross section is inversely proportional to the square root of the positron
kinetic energy. As long as the low energy cut-off is set sensibly, the stopping power error in the MCNP positron treatment can be kept within a few percents.

**Class I electron transport**

Class I algorithm (Figure 2.13) transports an electron with steps predetermined by energy losses. Usually, the loss at each step is chosen to be 8.3%:

\[ \frac{T_{\text{lost}}}{T_i} = 2^{-1/8} \quad \cdots \quad 2.41 \]

The electron path is thus broken down into major steps. Within each major step, the path is further divided into \( m \) sub-steps where \( m \) depends on the material in which the electron is transported. The default value for \( m \) ranges from 2 for \( Z < 6 \) to 15 for \( Z > 91 \) (Briesmeister 2000). The energy loss is fixed in advance, the distance that the electron will travel is determined by the CSDA with the collision stopping power:

\[ R_i = \int_{T_{\text{lost}}}^{T_i} \frac{dT}{S_{\text{col}}(T)} \quad \cdots \quad 2.42 \]

The collision stopping power includes the average energy loss by ionisation and excitation. However, ionisation is a stochastic event. It can cause sudden and large energy exchanges. Landau (1944) developed an energy straggling theory to account for this effect. It was subsequently modified by Blunck and Leisegang (1950). The small angular deflections from the atomic elastic interactions are modelled by a single accumulated deflection with the multiple scattering theory (Goudsmit and Saunderson 1940, Molière 1948). Bremsstrahlung production is based on Bethe and Heitler (1934) or one of its modern modifications (Seltzer 1988). The electron-electron scattering cross section comes from Seltzer (1988) or Møller (1932). If a separate treatment on positron is desired, one may use the Bhabha (1936) cross section for the positron-electron scattering.
To electron \( T_1 \) \( T_2, T_4 \)

bremsstrahlung photon

a sub-step

a major step

**Figure 2.13** Class I electron transport. An electron track is broken down into major steps and sub-steps with pre-determined energy losses. Secondary particles are produced at random locations within a sub-step. If the actual energy loss \( \Delta T \) is greater than the pre-calculated value, e.g., the pre-calculated loss is \( T_r-T_2 \) at the end of the second major step, then the next major step will start with an energy grid value \( T_4 \) corresponding to the actual loss. In this example, \( T_4 = T_1 - \Delta T \).

Because the electron is transported in an energy grid, there are two issues involved. One is that the electron energy is approximated by a grid value instead of using the “true” electron energy. A second, related issue is the strategy of assigning the appropriate grid value to the electron. MCNP allows the user to choose the default energy indexing or the so-called ITS\(^2\)-style energy indexing. A careful study of the MCNP electron transport subroutine *electr* shows that the default indexing scheme always assigns a grid value higher than the actual electron energy whereas the ITS-style indexing scheme assigns a grid value closest to the electron energy. Under the MCNP default scheme,

\[
T' = \begin{cases} 
T_0 & T = T_0 \\
T_i & T_{i+1} \leq T < T_i 
\end{cases}
\]

... 2.43

where \( T \) and \( T' \) are the original and the transport energy of the electron respectively; \( T_i \) and \( T_{i+1} \) are the \( i^{\text{th}} \) and the \( i+1^{\text{st}} \) energy grid values. On the other hand, the ITS-style scheme gives

\[
T' = \begin{cases} 
T_{i+1} & \text{if } T < \left( T_i + T_{i+1} \right)/2 \\
T_i & \text{otherwise}
\end{cases}
\]

... 2.44

\(^2\) ITS stands for Integrated TIGER Series (Halblieb and Mehlhorn 1984), an electron transport code incorporated into MCNP (Briesmeister 2000).
for $T$ in the energy bin $[T_{i+1}, T_i]$. Thus, the MCNP default indexing scheme assigns, on average, an energy half a group higher than the ITS-style scheme to the electron. Siebers et al (1999) found that the indexing scheme is affecting the bremsstrahlung production - sometimes overestimating the production and sometimes underestimating it. The ITS-style indexing provides a more stable production.

A criticism of the Class I electron transport is that the generation of secondary particles is not correlated to the state of the primary electron, i.e. the energy, position and the direction of the primary electron. They are generated entirely statistically although the actual electron energy is taken into account. Once the secondary particle production is determined from the appropriate cross section, the production site is sampled uniformly within the sub-step. For the same reasons, the energy deposited in the medium is not directly related to the state of the electron (Rogers and Bielajew 1990).

Energy loss straggling is one cause of the actual energy loss being greater than the pre-calculated loss. The electron can also lose a substantial portion of its energy in the bremsstrahlung production. Frequently, some corrections are necessary to bring the state of the primary track back into agreement with the actual energy loss (Figure 2.13). This is accomplished by skipping a few grid levels. The starting energy for the next step corresponds to the original grid energy minus the actual energy loss.

Another difficulty with the Class I algorithm is associated with the spatial boundary crossing. Whenever an electron crosses a geometry boundary, the energy grid must be set up again. Since the end of a major step or sub-step hardly coincides with the geometry boundary, small discrepancies in energy will result because the electron has not completed the track and it has not lost its energy as expected. If it is transported through many thin slabs, these errors will accumulate and become a major issue. Schaart et al (2002) suggested that the voxel size should not be less than 10 % of the CSDA range to minimise the boundary crossing error. Reynaert et al (2002) gave a more precise limit on geometry resolution: the minimum voxel size is

$$d = 0.85(1 - f)R_0$$

... 2.45
where \( f \) is the ratio in Equation 2.41 and \( R_0 \) is the CSDA range of the initial electron energy calculated with the total stopping power (Equation 2.42).

A similar situation is that an electron is skimming along a geometry boundary. The small angular deflections will bring the electron back and forth between two regions many times. The transport errors will again accumulate. Unfortunately, voxel size does not help here.

**Limitations of the multiple scattering theories**

Seltzer (1988) gives the following lower energy limits for a valid application of a multiple scattering theory:

<table>
<thead>
<tr>
<th>Material</th>
<th>Lower Energy Limit (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>low-Z</td>
<td>10–20</td>
</tr>
<tr>
<td>medium-Z</td>
<td>50–100</td>
</tr>
<tr>
<td>high-Z</td>
<td>100–200</td>
</tr>
</tbody>
</table>

*Table 2.4 Lower energy limit for multiple scattering theory (Seltzer 1988).*

These values constitute the lowest reasonable electron energy cut-off for a Monte Carlo calculation. Tracking of any electron below these energies may render the results questionable. A proper cut-off energy should reflect the likelihood of local absorption of the electron by the medium. It will keep the systematic error to a minimum and it will also speed up the calculation.

**Characteristic x-rays and Auger electrons**

Accompanying ionisation, may it be caused by a photon or an electron, is a cascade of characteristic x-ray and Auger electron emissions (atomic relaxation). However, the momentum transferred to the atom is large in the case of electron ionisation compared to photon ionisation. The atomic relaxation is largely ignored by MCNP in photon ionisation simply because most of the characteristic x-rays or fluorescence photons have energies below 100 kev (Figure 2.8). However, they may travel some distance before depositing their energies. They need to be tracked if their energy is
above the low energy cut-off. Contrary to MCNP(X), there is a low energy module in Geant4 (Agostinelli et al 2003) that takes care of the production of characteristic x-rays and the Auger electrons in photon and electron ionisations (Mantero et al 2005).

For a material with atomic number less than 12, all characteristic x-rays have energy below 1 keV which is the lowest possible energy cut-off for most Monte Carlo codes and the low energy limit in the cross section data. For the atomic number between 12 and 30 inclusively, there is only one characteristic x-ray photon with energy above 1 keV. From atomic number 31 onwards, the materials can emit two or more K characteristic x-ray photons above 1 keV.

An Auger electron is emitted when the characteristic x-ray photon energy is transferred to an orbital electron in a manner similar to the photoelectric absorption. The Auger electron energy is the photon energy minus the binding energy of the electron:

\[ T_{\text{Auger}} = h\nu - B_{\text{Auger}} \]  ... 2.46

For most Monte Carlo codes and their cross section data, only the K\(_\alpha\) (L\(\rightarrow\)K) and K\(_\beta\) (M\(\rightarrow\)K) characteristic x-ray photons are tracked. Therefore, the photon energy is assumed to be \(B_{K} - B_{L}\) where \(B_{K}\) and \(B_{L}\) are the average binding energies of the K and the L electrons. Also, the Auger electron is likely to be coming from the L shell. The Auger electron thus has energy\(^3\):

\[ T_{\text{Auger}} = B_{K} - B_{L} = B_{K} - 2B_{L} \]  ... 2.47

For uranium (Z = 92), \(B_{K}\) is about 116 keV and \(B_{L}\) is about 20 keV. \(T_{\text{Auger}}\) is about 76 keV. This is the highest Auger electron energy. For the vast majority of elements in medical physics applications (Z < 30), \(T_{\text{Auger}}\) is less than 10 keV and their energies are usually assumed to be deposited locally. Most Monte Carlo codes are capable of

---

\(^3\) The new MCNP electron library e/03 uses this approximation. The old library e\(l\) uses \(T_{\text{Auger}} = B_{K}\) which over-estimate the energy by 20–40% on top of the approximation discussed above because \(B_{L}\) is about 10–20% of \(B_{K}\).
tracking the Auger electrons. Whether they are tracked depends on the low energy cut-off. The tracking of the Auger electrons is also subject to the limitations of the multiple scattering theories. EGS4 ignores the Auger electrons entirely – their energies are too low for practical tracking in the materials that they are likely to occur.

Characteristic x-ray emission and Auger electron emission are competing processes. Their occurrence is determined by the characteristic x-ray yield that is defined as

\[ \omega_K = \frac{n_{\gamma,K}}{n_{+K}} \]

where \( n_{\gamma,K} \) and \( n_{+K} \) are the number of K characteristic x-ray photons and the number of K vacancies respectively. Auger electron emission is dominant in low-Z materials but characteristic x-ray emission is dominant in high-Z materials.

**Positron annihilation**

Positron annihilation may lead to the emission of one or several photons. Single-photon emission is extremely rare. The branching ratio of two-photon, three-photon and four-or-more-photon emission is about 1 : 2.7×10^{-3} : 1.5×10^{-6} (Charlton and Humberston 2001). Only two-photon emission is considered in all general purpose Monte Carlo codes. MCNP assumes that the annihilation occurs when the positron has lost all of its energy and the electron is at rest. Thus, the two photons are assumed to be exactly 180° apart with the first one emitted isotropically. EGS4 and other codes can account for the motion and the annihilation is in flight. The angle between the two photons is less than 180° due to the conservation of momentum.

**Tallies**

Perhaps the most basic quantity for a Monte Carlo code to calculate, or to tally, is the particle fluence that is number of particles crossing a unit area. ICRU Report 60 (ICRU 1998) provides two definitions of fluence:

\[ \Phi = \frac{dN}{dA} \]
and

\[ \Phi = \frac{dl}{dV} \quad \ldots 2.50 \]

where \( dN \) is the number of particles crossing the area \( dA \) that is perpendicular to the direction of the beam; \( dl \) is the total track length of the particles traversing the volume \( dV \).

Based on the two definitions and some analytical techniques, there are at least four types of estimators available in Monte Carlo works. In this work, only two types are employed – the analog and the track length estimators. They are described in the following sections. Other estimators, e.g. exponential track length estimator and next event estimator, can be found elsewhere (Williamson 1987, Briesmeister 2000)

**Analog estimator**

With the first fluence definition (Equation 2.49), one may actually count the number of particles. As soon as a particle enters a volume or crossing a surface, one is added to the tally. At the end of the simulation, we will have the total number of particles. Fluence is then derived. This simple counting strategy works fine even if the particles are statistically weighted. Very often, we artificially increase the number of particles that are likely to have significant contributions to the tallies; those with little contributions are tracked less frequently. Statistical weights are assigned to particles reflecting the artificial increase or decrease in their numbers. The contributions shall also be weighted accordingly. Thus, the total number of particles \( \hat{N} \) entering a volume and the fluence \( \hat{\Phi} \) are

\[ \hat{N} = \sum w_i \quad \ldots 2.51 \]
\[ \hat{\Phi} = \sum \frac{w_i}{A} \quad \ldots 2.52 \]

where \( A \) is the cross section area of the volume presented to the radiation beam. The total energy transferred \( \hat{E}_\nu \) and the kerma \( \hat{K} \) to the medium will be

\[ \hat{E}_\nu = \sum (w_i E_i - w_j E_j) \quad \ldots 2.53 \]
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\[ \hat{\Phi} = \sum \frac{w_i l_i}{V} \quad \text{... 2.55} \]

where \( w_i \) is the particle weight and \( m \) is the mass of the volume. \( \hat{N}, \hat{E}_\nu \) and \( \hat{K} \) are termed analog estimators. There are two main difficulties with \( \hat{E}_\nu \). First is that the particles traversing the volume without any interaction will not have any contribution to the tally (only \( p_1 \) in Figure 2.14 is contributing to the tally). Second is in the event that a rare but unimportant particle traversing with a collision, \( \hat{E}_\nu \) may be biased by the heavy weight. A lot of particles must therefore be tracked to counter-balance the bias. The convergence rate will be low.

A third difficulty associated with the analog estimator is subtler than the first two. It arises from the calculation of the area \( dA \) in the definition (Equation 2.49). Even the term ‘radiation beam’ is not necessary a well defined concept, especially when transporting particles in a highly scattering medium like electrons in water. The electrons cross the tally surface in all directions and it is difficult to have a definitive area for normalisation.

**Track length estimator**

The track length estimator of the fluence is based on the second ICRU definition (Equation 2.50).

\[ \hat{K} = \frac{\hat{E}_\nu}{m} \quad \text{... 2.54} \]

Every particle traversing the tally volume now contributes to the result (particles \( p_1, p_2 \) and \( p_3 \) in Figure 2.14).
Photon dose calculation

Besides fluence, another frequently used quantity in dosimetry is the photon kerma, kinetic energy released per unit mass. It is defined as

\[ K = \frac{dE_{kr}}{dm} \]  \hspace{1cm} (2.57)

where \( dE_{kr} \) is the energy released by the photon to a volume \( dV \) of mass \( dm \). From the definition of mass energy transfer coefficient (ICRU 1998),

\[ \frac{\mu_{kr}}{\rho} = \frac{1}{\rho} \frac{dE_{kr}}{d\ell} \]  \hspace{1cm} (2.58)

\[ \frac{dE_{kr}}{dm} = \frac{\mu_{kr}}{\rho} \frac{d\ell}{dm} \]  \hspace{1cm} (2.59)

\[ K = \frac{\mu_{kr}}{\rho} E \frac{d\ell}{dV} \]  \hspace{1cm} (2.60)

\[ K = \frac{\mu_{kr}}{\rho} E \Phi \]  \hspace{1cm} (2.61)

Thus, the kerma is directly linked to the photon fluence through the mass energy transfer coefficient. \( (\mu_{kr}/\rho) \) includes all energy transferred from the photon to the electron. A fraction \( g \) of the electron kinetic energy will be carried away through
bremsstrahlung. Only \((1 - g)\) of the initial transfer is absorbed by the medium. The mass energy absorption coefficient is

\[
\frac{\mu_{en}}{\rho} = \frac{\mu_{ir}}{\rho} (1 - g)
\]

... 2.62

The collision kerma is defined through the mass energy absorption coefficient:

\[
K_c = \frac{\mu_{en}}{\rho} E \Phi
\]

... 2.63

Calculating the kerma is relatively straightforward in Monte Carlo simulations because it is related to the photon fluence. The track length estimators usually give very reliable results. Calculating the dose, on the other hand, may not be as straightforward. Photon dose arises from a two-stage process. First the photon energy is transferred to an electron. This is what kerma calculates. Then the electron deposits the energy somewhere downstream. Because energy deposition is a stochastic process, the mass, or equivalently the volume, must be large enough to accommodate many energy deposition events and yet is small enough to be considered as deposition at a point for practical purposes.

The absorbed dose (ICRU 1998) is the mean energy imparted to the medium per unit mass

\[
D = \frac{d\bar{\varepsilon}}{dm}
\]

... 2.64

and the mean energy imparted is

\[
\bar{\varepsilon} = E_{in} - E_{out} + \sum Q
\]

... 2.65

where \(E_{in}\) and \(E_{out}\) are the total radiant energy entering and exiting the volume respectively; \(\sum Q\) is the net change in rest mass inside the volume. A positive \(Q\) value signifies a loss in rest energy and a negative one indicates a gain.

Under charged particle equilibrium (CPE), there is no net change in \(Q\) and the absorbed dose equals the kerma:
However, in the calculation of dose deposition in a water phantom, one must deal with the condition charge particle disequilibrium. It occurs in the dose build-up regions and in the beam penumbrae. A rigorous method is the use of an analog estimator that counts the energy in and out. As mentioned before, this method converges very slowly. In the simulation of a linear accelerator, there are simply not enough particles available. They are limited by computer storage, the largest integer and the length of the random number period. An alternative provided by MCNP is using the average energy deposited in the volume and the track length estimator of the fluence through the volume:

\[
\hat{D} = \hat{K}_c = \sum w_i I_i E_i (\mu_m / \rho) / V \quad \text{... 2.66}
\]

where \( H \) is the average energy deposition and it is termed heating number in MCNP.

### Precision and Accuracy

As in the case of physical measurement, Monte Carlo results have two types of associated errors – statistical and systematic (Figure 2.15). Statistical errors come from averaging a large number of events while systematic errors come from the modelling of the problem. Precision describes how small the statistical error is. The smaller the statistical error is, the higher the precision we have. Similarly, high accuracy means small systematic error. It describes how close the calculated value is to the true value.
The accuracy of a calculation is difficult to quantify. There are many factors affecting the calculation. The code may have software bugs. The physics models contain certain simplifications. The cross section data have uncertainties associated with them. How the Monte Carlo code samples the cross section data may also introduce some systematic errors. Some of these systematic errors have already been addressed in previous sections on radiation transports and their cross section data. Finally, the user will inadvertently introduce some errors from the approximations in the geometry and in the material compositions.

The precision of a calculation is much easier to ascertain than the accuracy. It is the consequence of statistical fluctuations and therefore follows the rules of statistics. In particular, the laws of large numbers and the central limit theorem govern the behaviour of the tally that is accumulating contributions from a large number of independent events.

During the transport of a particle (a history), its contribution to the tally (result) will be accumulated. The tally could be the energy deposition in a detector, the particle fluence crossing a volume or any other quantity of interest. Since the random numbers from a good generator do not exhibit correlation among them, the particle histories are independent events. Suppose \( x_i \) is the contribution by the \( i^{th} \) of \( N \) histories, the collection \( X = \{ x_i \} \) of these contributions will have a history score PDF \( f(x) \) which is usually unknown. If the true mean (in a statistical sense) exists, the strong law of large numbers asserts that the sample mean \( \bar{x} = \frac{\sum x_i}{N} \) will converge to it for a sufficiently large \( N \) or, in other words, if the simulation is long enough.
It is important to bear in mind that the random number generator imposes a finite period on the random numbers. The practicality of having a “long enough” simulation is often limited in some complex calculations. Some variance reduction techniques are often required to promote the rate of convergence.

The central limit theorem asserts that if \( \mu = E(X) \) exists then the random variable \( X \) will conform to the normal distribution:

\[
\lim_{n \to \infty} \frac{X - \mu}{\sigma / \sqrt{N}} = N(0, 1)
\]

where \( N(a, b) \) denotes the normal distribution with mean \( a \) and standard deviation \( b \); \( \sigma \) and \( N \) are the standard deviation and sample size of \( X \) respectively. The standard error or standard error of the mean, is then given by

\[
\sigma_X = \frac{\sigma_X}{\sqrt{N}}
\]

where \( N \) is the sample size. \( \sigma_X \) is a measurement of the variability of the estimated mean similar to \( \sigma_X \) being a measurement of the variability of the sample values. The confidence level can thus be estimated from a standard normal distribution table; one can find that the probability of \( \bar{x} \) within \( 1\sigma_X \) from the true mean is 68.26 %, within \( 2\sigma_X \) is 95.44 %, the 95 % confidence level is \( \mu \pm 1.96\sigma_X \), etc.

**MCNP statistical tests**

For each tally \( \bar{x} \), MCNP automatically calculates and prints out the associated relative error which is defined as

\[
\text{Unless stated otherwise, } \mu \text{ and } \sigma \text{ will no longer take on the meaning of linear attenuation coefficient and cross section from this point onwards. Instead, they will assume the meaning of mean value and standard deviation respectively.} \]
\[ R = \frac{\sigma_x}{\bar{x}} \]

Since \( \sigma_x \) is inversely proportional to \( \sqrt{N} \), it is necessary to increase the number of histories by threefold in order to halve the relative error. The computing time shall also be increased threefold. This is the inherent drawback of Monte Carlo calculations – the computing power hungry nature of the method. Coming with the tally, MCNP also provides a set of ten statistical tests. These tests are designed to establish the reliability of the results. They include

1. random behaviour of the mean
2. relative error
   a. magnitude
   b. monotonically decreasing
   c. decrease by \( 1/\sqrt{N} \)
3. variance of variance
   a. magnitude
   b. monotonically decreasing
   c. decrease by \( 1/N \)
4. figure of merit
   a. constant
   b. random behaviour
5. slope of history score PDF

The following discussions are summarised from the MCNP4C2 manual (Briesmeister 2000).

**Mean**

As discussed in previous section, the mean is a random variable of averaging a number of tally contributions. In fact, the theorem predicts that these fluctuations will conform to a normal distribution. Thus, the fluctuation must take on random values. This implies that the mean value should exhibit random behaviour as the number of histories increases. MCNP tests for the randomness of the mean during the last half of the simulation.
Relative error

The experience of the MCNP developers suggests that a reliable result should have a relative error less than 0.05 for a point detector tally and it should be less than 0.1 for other detector tallies. As noted in previous sections, the relative error $R$ decreases by $1/\sqrt{N}$.

Variance of variance

The variance of variance (VOV) is the measurement of the “error of the error.” Analogous to the relative error $R^2$ which is a measure of the error of the mean, the VOV is a measure of the error of $R$. It is defined as

$$VOV = \frac{\sigma_R^4}{\sigma_x^4} = \frac{1}{N} \left[ \sum (x_i - \bar{x})^4 \right] - 1$$

where $\sigma_R$ is the standard deviation of the relative error and $\sigma_x$ is the standard deviation of the mean.

The VOV should be decreasing as $1/N$ implying that $\sigma_x$ will become a stable finite value for large $N$. It is an important quantity because it ensures that the sample standard deviation $\sigma_x$ is a good estimation of the true variance $\sigma^2$ and that the central limit theorem is applicable.

Figure of merit

The figure of merit (FOM) estimates the efficiency of a calculation. It is defined as

$$FOM = \frac{1}{R^2 T}$$

where $R$ is the relative error and $T$ is the computing time. Since $R$ is inversely proportional to $\sqrt{N}$ and $T$ is proportional to $N$, the FOM should nearly be a constant over $N$. If the FOM is not a constant at the later half of the simulation, the tally is not giving a reliable result. Also, the larger the FOM value is, the more efficient the simulation is.

Slope of history score PDF

The slope $m$ of the history score PDF is arguably the most important test in a simulation. A value greater than 3 indicates a true convergence of $\bar{x}$ to the true mean. Otherwise, it could be a false convergence and the result cannot be trusted.
The central limit theorem requires that $\mu = E(X)$ exists. MCNP assumes that an adequately sampled $f(x)$ will eventually decrease faster than $1/x^3$ for large $x$ and therefore, both $\int_{-\infty}^{\infty} xf(x) \, dx$ and $\int_{-\infty}^{\infty} x^2 f(x) \, dx$ will exist.

![Figure 2.16 Pareto fit of the largest tally values. $f(x)$ will eventually decrease faster than $1/x^3$. A Pareto fit is carried out for the largest 250 tally values. The slope of $f(x)$ is then estimated from $f_{\text{Pareto}}(x)$.]

Thus, the slope is the $m$ in $1/x^m$ in the region of large $x$. To calculate $m$, MCNP carries out a Pareto fit with parameters $a$ and $k$ to the frequency of the largest 250 tally scores (Figure 2.16):

$$f_{\text{Pareto}}(x) = a^{-1} \left( 1 + \frac{kx}{a} \right)^{-\frac{1}{k+1}}$$

... 2.73

Then,

$$m = \frac{1}{k} + 1$$

... 2.74

The Pareto function is used because it can approximate the shapes of a large variety of functions – from a constant function to exponential functions.
Chapter 3  Medical Linear Accelerators and Their Simulations

Externally, a linac system consists of a couch for the patient, which is adjustable in height and can be rotated horizontally, and a rotating gantry housing the treatment head where the radiotherapy beam is shaped and delivered to the patient. The combined movements of the couch and the gantry allow the radiotherapy beam to be delivered at practically any angle to the patient. Hidden from view is the mechanism generating and accelerating the electrons to the required energy, and conversion of the electrons into bremsstrahlung photons (Figure 3.1).

Figure 3.1  The schematic drawing of some major components inside a linac (Schlegel and Mahr 2002).
**Basic working principles**

The electrons are injected from an electron gun into the accelerating waveguide which accelerates the electrons to the required energy. The waveguide is powered by microwave in the form of either travelling wave or standing wave. The microwave is generated by a klystron or a magnetron. In both mechanisms, a high current of low-energy electrons is injected into resonance cavities to create the 3 GHz microwave. The choice of klystron or magnetron depends largely on pragmatic grounds: a klystron is larger in size and operates at lighter voltage than a magnetron — a magnetron can fit into the rotating gantry whereas a klystron must be fitted behind the gantry requiring a special rotating joint to transmit the microwave. A series of waveguides feed the microwave into the accelerating wave guide.

With a travelling wave accelerator, the microwave is fed through an aperture at one end of the accelerating waveguide and exit at the other end (Figure 3.2a). The travelling microwave generates a travelling electric field and the electrons “surf” on this moving field. Electrons at different position in the field receive greater or smaller pushes so that they are bunched together (Figure 3.2b). As the electrons gain energy and speed, the speed of the electric field must be adjusted accordingly.

![Figure 3.2 Travelling wave guide (Greene and Williams 1997).](image-url)
On contrary, the standing wave accelerator reflects the wave at both ends with a \( \pi/2 \) phase change to build up a standing wave. Thus the microwave can come in through any cavity. The push is accomplished by the phase shift. As the anti-node turns from negative amplitude to positive, it will give the electrons a push (Figure 3.3a and b). Thus every anti-node cavity has a chance to accelerate the electrons. With a clever arrangement, the node cavities can be coupled to the side and shorten the length of the whole structure (Figure 3.3c).

![Figure 3.3 Standing wave guide (Greene and Williams 1997).](image)

Most modern linacs have the accelerating waveguide inside the horizontal arm of the gantry. A bending magnet is required to steer the horizontal accelerated electron beam to a vertical one for delivery. The structure turns the beam by 90° or 270°.

The trajectory of an electron going through a 90° bending magnet depends on its energy and its displacement from beam axis. Higher-energy electrons are bent less than the lower-energy ones. Electrons farther away from the beam axis will have a longer path length in the longitudinal direction — in the direction parallel to the pole face. Thus the focal spot on the tungsten target is usually elliptical rather than circular (Figure 3.4a).
The achromatic property of a 270° bending magnet focuses the electrons to the focal spot independent of the electron energy. The higher-energy electrons travel deeper into the magnet system and are subjected to a stronger magnetic force; the high- and low-energy electrons emerge at the same point and in the same direction (Figure 3.4b). This is the advantage of a 270° bending magnet over the 90° ones. The disadvantage of a 270° bending magnet is in its size. A linac with a 270° bending magnet needs more headroom.

Philips Elekta developed the slalom travelling accelerator for their SL series linacs (Figure 3.5). It uses bending magnets to turn the accelerating electron beam inside the slalom waveguide. This design shortens the waveguide structure and lowers the height of the gantry. Along the waveguide, there are two 45° bending magnets on opposite sides of the waveguide. Together they act as the first part of the 270° bending magnet. Electrons of different energies are positioned differently for their entry into the final 112.5° turn. Although the final bending magnet is 112.5°, the electrons go through a total bend of 202.5°. This system has the achromatic property of a 270° bending magnet and a small dimension as a 90° bending magnet (Botman et al 1985).
The above is a very brief description of the working principle of a linac system. There are many auxiliary systems to facilitate the generation and the acceleration of the electron beam, e.g., modulator to regulate the microwave pulses, cooling system, vacuum system, etc. Fuller descriptions can be found in Greene and Williams (1997) and Metcalfe et al (1997).

**Treatment head**

The treatment head is housed at the end of the rotating gantry. It shapes and delivers the therapeutic beam to the patient. In the case of an electron therapeutic beam, the accelerated electron beam is directed towards a scattering foil to give a flat beam profile. In the case of an x-ray therapeutic beam, the initial electron beam will strike on a tungsten target to create a beam of bremsstrahlung x-rays which will go through a flattening filter. Therefore, an intricate interlock system for exchanging components for different treatment regime and a monitoring system are essential to safeguard any mishaps. Figure 3.6 shows the major components in the Philips Elekta SLi treatment configured for 6 MV beam. This work drawing is the reference during the construction of the geometry, making measurements and comparing the calculated and measured dose profiles. The detail dimensions and material compositions are proprietary information and they shall not be disclosed.
Figure 3.6 Major components in the Elekta SLi treatment head and the coordinate system. The coordinate system follows ICRU Report 42 (ICRU 1987). The collimator angle in the diagram is 90° so that the inline scan corresponds to a scan along the y-axis and the crossline scan along the x-axis. The lower diagram shows the cross-sectional shape of a pair of MLC leaves as modelled in this thesis. All diagrams are not drawn to scale.
Initial electron beam

The initial electron beam is the terminology of ICRU Report 42 (ICRU 1987). It is the beam of the accelerated electrons impinging onto the tungsten target. From the electron gun to the tungsten target in the treatment head, the electron beam must operate in a near vacuum condition which is less than $1.5 \times 10^{-5}$ Pa (p48, Greene and Williams 1997). In a Monte Carlo model, it is generally assumed that the initial electron beam hits the target in a perfect vacuum. Also, it is assumed that the beam direction is orthogonal to the target surface and it hits right at the centre of the target. In reality, the beam drifts off from the target centre and it may not strike perpendicularly. Monitoring and correcting the beam parameters are among the functions of the monitor chamber.

Strictly speaking, an $x$ MV photon beam means that it is a bremsstrahlung photon beam coming from the stopping of the $x$ MeV electrons. Therefore, the initial electron beam energy should be $x$ MeV and so is the maximum photon energy. However, the penetration power of the photon beam depends on the mean electron energy, the target thickness and its atomic number, the design of the flattening filter and the field size. It was found that machines of the same MV but of different makes gave very different percentage depth dose curves and British Institute of Radiology Supplement 25 (BIR 1996) adopts the concept of nominal MV to characterise the photon beam. Thus, a photon beam is called an $x$ MV beam if it produces a percentage depth dose curve similar to that in BIR Supplement 25. As a result, the initial electron beam energy may not have the same value as the nominal energy.

Since the initial electron beam is fined-tuned during commissioning, on-site in the hospital, the manufacturer’s supplied parameters may not be applicable to a specific machine. For the 6 MV beam of the Elekta SLi machine, the manufacturer suggests that the initial electron beam has mean energy 6 MeV, 1 MeV full-width-at-half-maximum (fwhm) and its spot size is 1 mm fwhm. These values represent the starting point of the series of trial and error simulations. The values that give the best match between the simulated dose distribution and the measured one are adopted as the correct parameter values. The fine-tuning of the initial electron beam will be discussed further in a later section on the actual Monte Carlo simulation of the Elekta SLi linac.
**Target block**

The electron target is a circular disc, 2 mm (diameter) × 1 mm, of 85% tungsten alloy. A copper alloy back-up plate is holding the target in place and dissipates the heat generated by the stopping of the initial electron beam. At 6 MeV, the electron CSDA range in tungsten is about 2 mm. Since the target is thinner than the CSDA range, some electrons are not stopped in the target and the bremsstrahlung generation is less than maximum. Furthermore, leakage of contaminant electrons into the photon beam is inevitable. A thicker target will decrease the amount of contaminant electrons but it will also soften the emitted bremsstrahlung photon spectrum. Thus the target thickness is a compromise among the emission spectrum, the bremsstrahlung generation efficiency and the amount of contaminant electrons.

Due to the presence of the back-up plate, most of the contaminant electrons leaking from the target are removed. To minimise the attenuation of the bremsstrahlung photon by the back-up plate, copper is chosen for its lower atomic number.

**Primary collimator**

The primary collimator is a circular tungsten alloy block with a cone-shape opening at the middle. Its function is to prevent leakage of the bremsstrahlung photon in unwanted directions. The cone angle is about 28° which projects a 50 cm diameter circle on the isocentric plane, 100 cm from the target centre. This also means that the bremsstrahlung beam is about 50 cm at 100 cm source-to-surface distance (SSD) if secondary collimation, e.g. jaws, diaphragms and multileaf collimators, is not present. This represents the maximum possible field size.

**Flattening filter**

Beneath the primary collimator is the flattening filter. The bremsstrahlung beam is emitted mainly in the forward direction and the photon energy is almost independent of the emission angle. This gives rise to a high dose at the central axis and the dose falls off quickly with respect to the off-axis distance. The profile of the flattening filter is roughly conical (Figure 3.7) to attenuate the photons more near the central axis so that the dose profile is relatively flat at 10 cm deep in water at 100 cm SSD.
The flattening filter is usually made of aluminium because its attenuation coefficient is relatively flat over a wide range of energies (Figure 3.8a). This minimises the preferential absorption of high-energy photons. However, for the range of energies of a 6 MV beam, iron and copper are better materials for the flattening filter. Both materials show a flatter curve than aluminium and tungsten (Figure 3.8b). When the material density is also taken into account, i.e., when the linear attenuation coefficients are considered, each curve will be shifted upwards by a factor of the corresponding material density. Thus, copper has higher attenuation than iron but the shape of the curve remains. Elekta has chosen steel over copper as their material for the construction of the 6 MV flattening filter.
**Monitor chamber and backscatter plate**

The monitor chamber serves two main purposes: (1) to monitor the energy, position and incident angle of the initial electron beam; and (2) to monitor the radiation output from the machine. The significance of the first function is in the uniformity of the dose delivery whereas the second function provides the information on how much dose is being delivered.

The monitor chamber is actually composed of two or more parallel-plate multi-channel ionisation chambers. The chambers are separated by thin Mylar films coated with carbon to act as electrodes. The ratio of the signals from different channels provides the information on the beam position and incident angle. The information is fed back to the bending magnet so that the magnetic field is adjusted for spatial and/or angular steering of the initial electron beam. The integration of the signal from all channels in one chamber gives the number of monitor units (MU) which is calibrated so that 1 MU is equal to 1 cGy at the depth of maximum dose in a 10×10 cm² field at 100 cm SSD.

Since there are electrons and photons backscattered from the secondary collimators to the monitor chamber, the induced current will give rise to incorrect monitor readings. The strategy for placing the monitor chamber in the treatment head is simply to put it as far away from the secondary collimators as possible. To eliminate the backscattered particles, the Elekta linac has a 3 mm thick aluminium plate installed beneath the monitor chamber to absorb the backscattered particles. Hounsell (1998) investigated and found that the plate is necessary and effective.

**Multileaf collimator**

The multileaf collimator (MLC) is the most important component in conformal radiotherapy and intensity modulated radiotherapy (IMRT). In conformal radiotherapy, it shapes the beam to the outline of the tumour. More precisely, the beam conforms to the outline of the planning target volume (PTV) which includes the tumour itself, the spreading of the tumour cells to its neighbouring tissues and the effect of organ movement. In IMRT, the individual leaves of the MLC also moves into various positions to create a fluence map conforming to the three-dimensional contour of the PTV. Thus, each MLC leaf
must have a narrow foot-print when projected onto the isocentric plane;
- must provide sufficient attenuation to the portion of the bremsstrahlung beam outside the field; and
- must introduce as little scattering into the beam as possible.

The leaf is doubly focused, meaning that it has a cylindrical tip and a tapered body focused at the target (Figure 3.6 and Figure 3.9). Since there is a gap between two leaves, radiation leakage is inevitable. To minimise the leakage, a step is introduced to the two sides of the leaf. The step also makes the leaf width differ from the pitch. The Elekta SLi MLC leaf has a 1.1 cm width and 1 cm pitch projected at the isocentre (Hounsell and Jordan 1997). Figure 3.9 illustrates the meanings of leaf width and leaf pitch. Measurement of a single leaf by Jordan and Williams (1994) found that the width in water phantom at 50 % dose is 0.97 cm at 6 MV and 0.91 cm at 20 MV due to the difference in the scattered radiation at the two energies.

![Figure 3.9](image)

*Figure 3.9 The shape of a leaf and the definition of width and pitch. The drawing is not to scale and the degree of tapering is highly exaggerated for clarity.*

A flat leaf tip gives the smallest penumbra if it is focused at the target. This will require the leaves moving along an arc centred at the target. The tight space available inside the treatment head may not allow such an elaborate movement and its control. The cylindrically shaped tip represents a compromise between design and performance. Although the penumbra degrades with the curved design due to partial transmission, it does allow the leaf to move linearly in and out of the field while the
penumbra remains relatively constant (±1 mm at the depth of maximum dose, Jordan and Williams 1994). The leaf is about 7 cm thick, made of tungsten alloy. The transmission of the primary beam through the leaf's full thickness is about 1%. The leakage between leaves is in the range of 2–3% (Huq et al 1995, Hounsell and Jordan 1997).

In the Elekta SLi linac, there are 40 pairs of MLC leaves in two banks. All leaves in the same bank have the same shape and those in the opposite bank are their mirror image. Therefore, the leaves in one bank are aligned along an arc that centres at the target. Under this geometry, the leaves away from the central axis plane have larger width and larger pitch on the isocentric plane than the central ones.

In the MCNPX model of the MLC, a pair of leaves is constructed at the central axis as in the left drawing in Figure 3.9. They are then rotated by $\theta/2$ to obtain the two central pairs. The angle $\theta$, about 0.57°, is the angle subtended by the leaf pitch at the target (the right drawing in Figure 3.9). Each pair of leaves further away from the central axis plane is rotated by an additional $\theta$. The finished MLC geometry is plotted in Figure 3.10.

![Figure 3.10 A bank of 40 MLC leaves from the MCNPX geometry plot.](image)

**Diaphragms**

Additional shielding of the radiation field is provided by two sets of diaphragms in the Elekta SLi linac. Right beneath the MLC are the $y$-diaphragms. They move...
linearly in the same direction as the MLC leaves but only 3 cm thick. Further downstream are the x-diaphragms which move orthogonally to the MLC leaves and the y-diaphragms. The x-diaphragms have the same thickness as the MLC leaves, about 7 cm. To create an irregular field, the diaphragms are so positioned that they give the smallest rectangular field enclosing the PTV while the MLC leaves are extended into the field to shield the tissue outside the PTV. Figure 3.11 illustrates the principle of the working relationship between the MLC and the diaphragms.

![Figure 3.11 The positioning of the MLC leaves and the diaphragms in the beam's eye view.](image)

**Mirror and screen**

The mirror is a thin Mylar film coated with aluminium to reflect a light field onto the patient for positioning. The screen is also made of Mylar film without coating. Its main function is to prevent objects being dropped into the treatment head. For the low attenuation presented to the bremsstrahlung beam by the Mylar film, the mirror and the screen are usually not included in simulations. However, both components are modelled in this work for accuracy.

**MCNPX geometry of the Elekta SLi**

The geometry of the completed model is plotted in Figure 3.12. All components shown in Figure 3.6 are included. Also plotted are two output planes where particle data are written to surface source files and in particular, output plane 1 between the monitor chamber and the backscatter plate is where phase space models are created.
Figure 3.12 The Elekta SLi linac model in MCNPX. The "hole" in the target block is the electron window for an electron therapeutic beam. The electron target for the photon therapeutic beam and the details of the monitor chamber are too small to be shown. The two output planes are the positions where particle data are recorded. The left figure is a plot on an xz-plane (y=0) and the right figure is on a yz-plane (x=0).
**Simulation of a linac**

The Monte Carlo method is generally accepted as the most accurate method in predicting the radiation field generated by a linac, and quantities arising from this field (Wong and Purdy 1990, Mackie et al 1994, Mackie et al 1996, DeMarco et al 1998, Mohan 1997, Ma and Jiang 1999, Andrea et al 2001, Verhaegen and Seuntjens 2003). It can provide valuable data that is difficult or impractical to measure (Andrea 1991). Since a Monte Carlo simulation of the treatment head of a linac can be very time consuming, it is common practice to break the simulation into steps such that the results from one step become the input to the next. Thus, a simulation is carried out in three steps – the transport through the patient independent components, the transport through the patient-specific components and the transport through the air column into the water phantom/patient.

In the first step, the initial electron beam is brought into interaction with the target and a shower of bremsstrahlung photons and contaminant electrons is generated. These particles are transported through the primary collimator, flattening filter and the monitor chamber. All particles emerging from the monitor chamber are recorded on output plane 1 to create a surface source file. The head components from the target to the monitor chamber are patient-independent because the phase space remains the same regardless the settings of the beam modifiers – the multileaf collimator and the x- and the y-diaphragms. Once the simulation of these patient-independent parts is complete, the same surface source file can be used for further simulations downstream with different beam modifier settings. Significant simulation time can thus be saved from this simple procedure.

A preliminary simulation, without variance reduction technique, of this patient-independent part with 500 million incident electrons with mean energy 5.8 MeV and 1 MeV fwhm shows that only 24 million photons and 0.3 million electrons are recorded in output plane 1. This represents 1.2 % of the all photons produced. 98.8 % of the photons are lost in the process mostly through photoelectric absorption. This simulation took 6.5 days with a Pentium 4, 2.2 GHz computer. The following table is summarised from the MCNPX output file:
Table 3.1 Simulation summary of the patient-independent part of the linac. The escaped photons includes all photons leaving the geometry. Only a fraction of these photons pass through the output plane and being recorded. The photon energy cut-off is 10 keV.

A second stage simulation transports the photons and electrons through a 20×20 cm² field to output plane 2, again without variance reduction techniques. There are only 3 million photons and less than 25 thousand electrons are recorded in output plane 2; that is, only 12.5 % of the photons in output plane 1, or 0.15 % of all the bremsstrahlung photons generated in the first stage, emerge from the treatment head. Again as in the first stage, most photons are absorbed due to photoelectric effect. Table 3.2 is the summary of the simulation:

Because of the low number of particles in output plane 2, further simulation into the water phantom does not produce reasonable results. An attempt with voxels as large as 5.0×0.5×0.5 cm³ produces relative errors about 3 % inside the field and over 30 % outside the field (Figure 3.13). The fluctuation between -10 and -5 cm in the figure suggests that under-sampling or correlated histories are present in the simulation. Under-sampling is probably due to the complex geometry of the MLC leaves in the

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Table 3.2 Simulation summary of a 20×20 cm² field. Comments for Table 3.1 is also applicable here.
second stage simulation. The first stage is likely to be well sampled but the number of particles in the surface source file is simply insufficient for the second stage simulation. Correlated histories occur when two or more histories start with the same random number. Therefore the histories are exactly the same and the variance is underestimated. It is clear that variance reduction techniques are of absolute necessity.

Figure 3.13 Dose profile from the preliminary simulation without VRT. Both measurement and MC calculated data are normalised to 1 at CAX. The fluctuation makes the MC normalisation questionable. Therefore, comparison with measurement is not meaningful.

Three variance reduction techniques are considered – geometry splitting/Russian roulette, bremsstrahlung splitting and reuse of phase space particles. As explained in Chapter 2, geometry splitting/Russian roulette artificially increases the number of particles in the direction specified by the user and randomly terminates some of those travelling in reverse. Thus, the particles can be “pushed” towards the patient-end of the treatment head. Some authors had investigated the technique in combination with
bremsstrahlung splitting and concluded that they should be used with caution in the linac simulations (e.g., Kawrakow et al 2004, Chin 2005). The combination tends to under-sample electrons in important regions (both spatial and in energy). The resulting dose profile in the water phantom exhibits large fluctuations but with small relative errors. Sempau et al (2001) coined the term “latent variance” for this phenomenon.

On the other hand, bremsstrahlung splitting is needed for two reasons. Reducing the in-field relative errors to 1.5 % will require 2 billion source electrons. As already shown by the preliminary simulation, this means one month of simulation time for the first stage. Yet, it does not guarantee that there are sufficient particles in the surface source file for a well-sampled second stage simulation. Secondly, there are only a finite number of random numbers. Keep increasing the number of source particles will inevitably cause correlated histories. The third reason is due to the way MCNPX handles the reusing of particles in a surface source file. The number of times, \( n \), that a particle is reused is specified in the \( NPS \) card. Roughly speaking, \( n \) is the \( NPS \) value in the current run divided by the \( NPS \) value in the original run. Unfortunately, the largest allowable integer in MCNPX is about 2.1 billion\(^5\). Therefore, the \( NPS \) value of 500 million in the preliminary simulation has practically ruled out the reuse of particles.

The preliminary simulation of the bremsstrahlung beam from the initial electron beam of 5.8 MeV mean energy in a 20×20 cm\(^2\) field is carried out again with bremsstrahlung splitting and particle reuse. In the first stage simulation with 15 million source electrons, bremsstrahlung splitting is set to 20 (usually between 20 and 100, Kawrakow et al 2004). In the second and third stages, each particle in the corresponding surface source files is reused 10 times. Figure 3.14 is the resulting dose profile:

\(^5\) The 3\(^{rd}\) release of MCNP5 does allow integers close to \( 10^{20} \) and the random number period up to about \( 10^{19} \) (Goorley and Olsher 2005).
Figure 3.14 Dose profile with VRT. VRT clearly improves the sampling and the fluctuation is lessened. Normalisation at CAX is not as much a problem as in Figure 3.13. Comparison between calculation and measurement becomes possible.

**Fine-tuning the initial electron beam parameters**

As already pointed out earlier in this chapter, the nominal energy is not a reliable indication of the initial electron beam energy. Although the manufacturers usually provide very accurate data on the dimensions of the head components, their initial electron beam parameters – the energy spectrum, the dimension of the beam and the angle of the beam hitting the target – may not be correct for simulations. One reason is that a linac is very often fine-tuned to match an existing linac during commissioning and therefore, the manufacturer’s data may not accurately reflect the parameters for that particular machine. Perhaps a more important reason is related to the combination of simplifications in the geometry and the material composition of the head components and the assumptions about the initial electron beam in the simulation: some authors assume a monoenergetic beam; others assume a pencil beam of zero diameter; whereas yet others assume a simple cone as a flattening filter; and so on and so forth. Besides, different Monte Carlo codes may use different
physics models and interaction cross section library. They therefore have different bremsstrahlung yields, different back scattering properties, etc. Thus it is up to the authors to fine-tune their initial electron parameters to offset various systematic errors in the modelling of the linac.

Although some authors use the manufacturer's data directly for their simulations (e.g. van der Zee and Welleweerd 1999), it is more common to recover these parameters by matching the calculated percentage depth dose (PDD) curve and the off-axis dose profiles in water with the physically measured ones (Lovelock et al 1995, DeMarco et al 1998, Fix et al 2001a, Fix et al 2001b, Lin et al 2001, Hartmann Siantar et al 2001, Ding 2002, Sheikh-Bagheri and Rogers 2002b). There is a wealth of literature in the Monte Carlo simulation of the linacs but very few authors report all the simulation parameters. Table 3.3 summarises some of these values found in the literature.

Verhaegen and Seuntjens (2003) suggest the following strategy for fine-tuning the initial electron parameters in a water phantom:

---

**Step 1. Energy spectrum:**
- Use monoenergetic beam at nominal energy or manufacturer’s specification on the beam’s mean energy and its fwhm.
- Compare PDDs in 10×10 cm² field.
- Normalisation at a depth at least 10 cm deep to avoid statistical uncertainties near surface.
- Vary the energy for the best match with measurements.

**Step 2. Radial distribution:**
- Use 2 mm fwhm as an initial guess or manufacturer’s specification.
- Compare lateral dose profiles in a large field.
- Should be carried out in air or at shallow depth to reduce influence from phantom scatter.
- Vary the beam radius or fwhm for best match

**Step 3. Verify and repeat steps 1 and 2 if necessary.**
<table>
<thead>
<tr>
<th>Model</th>
<th>Nominal energy (MV)</th>
<th>$e^-$ beam energy mean (fwhm) (MeV)</th>
<th>$e^-$ beam geometry (mm)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elekta SL15</td>
<td>10</td>
<td>9.5 (--)</td>
<td>2.0†</td>
<td>van der Zee and Wellesweerd 1999</td>
</tr>
<tr>
<td>Elekta SL25</td>
<td>6</td>
<td>6.8 (--)</td>
<td>1.5†</td>
<td>DeMarco et al 1998</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>10.4 (--)</td>
<td>1.5†</td>
<td></td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>22.0 (--)</td>
<td>1.5†</td>
<td></td>
</tr>
<tr>
<td>Elekta SL25</td>
<td>6</td>
<td>6.3 (1.071)</td>
<td>1.1†</td>
<td>Sheikh-Bagheri and Rogers 2002a</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>19.0 (0.950)</td>
<td>1.0†</td>
<td></td>
</tr>
<tr>
<td>Elekta SLi</td>
<td>6</td>
<td>6.0 (1.0)</td>
<td></td>
<td>Bramoulé et al 2000</td>
</tr>
<tr>
<td></td>
<td>18</td>
<td>17.0 (1.0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>21.0 (1.0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Elekta SLi</td>
<td>6</td>
<td>6.8 (1.0)</td>
<td>2.0†</td>
<td>Haryanto et al 2002</td>
</tr>
<tr>
<td>Siemens KD</td>
<td>6</td>
<td>6.8 (0.952)</td>
<td>3.2†</td>
<td>Sheikh-Bagheri and Rogers 2002a</td>
</tr>
<tr>
<td></td>
<td>18</td>
<td>14.7 (2.058)</td>
<td>1.0†</td>
<td></td>
</tr>
<tr>
<td>Varian (low energy)</td>
<td>4</td>
<td>3.7 (0.12)</td>
<td>1.5†</td>
<td>Sheikh-Bagheri and Rogers 2002a</td>
</tr>
<tr>
<td>Varian (high energy)</td>
<td>6</td>
<td>5.7 (0.171)</td>
<td>2.0†</td>
<td>Sheikh-Bagheri and Rogers 2002a</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>10.5 (0.315)</td>
<td>1.5†</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>14.5 (0.435)</td>
<td>1.7†</td>
<td></td>
</tr>
<tr>
<td></td>
<td>18</td>
<td>18.3 (0.549)</td>
<td>1.1†</td>
<td></td>
</tr>
<tr>
<td>Varian 600C</td>
<td>6</td>
<td>5.8 (--)</td>
<td></td>
<td>Lovelock et al 1995</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>15.4 (--)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Varian 2100C</td>
<td>6</td>
<td>5.8 (--)</td>
<td></td>
<td>Marinos 1999</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>6.0 (--)</td>
<td></td>
<td>Chin 2005</td>
</tr>
<tr>
<td>Varian 2100BX</td>
<td>6</td>
<td>6.02 (1.0)</td>
<td>1.2†</td>
<td>Ding 2002</td>
</tr>
<tr>
<td></td>
<td>18</td>
<td>18.00 (1.0)</td>
<td>1.5†</td>
<td></td>
</tr>
<tr>
<td>Varian 2300C/D</td>
<td>6</td>
<td>6.05 (--)</td>
<td>2.0†</td>
<td>Fix et al 2001a</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>15.0 (--)</td>
<td>3.0†</td>
<td>Fix et al 2001b</td>
</tr>
</tbody>
</table>

Table 3.3 Some initial electron beam parameters used in the literature. The beam is assumed to be monoenergetic when the fwhm of the energy distribution is not quoted.

- pencil beam of zero diameter.
- uniform beam – diameter not provided by author.
- uniform beam – stated figure is the beam diameter in mm.
- Gaussian beam – stated figure is the beam fwhm in mm.
In this work, two fields — 10×10 cm² and 20×20 cm² — are simulated and compared with measurements. The initial electron beam energy is varied from 6.0 MeV to 6.6 MeV, each with 1 MeV full width at half maximum. The beam is uniform and it strikes the electron target at right angle. The spot size is 1 mm in diameter. Off-axis dose profile at depth of maximum dose and the PDD curve are calculated. The scoring voxels for the dose profiles have dimension 5.0×0.5×0.5 cm³ while those for the PDDs are 1.0×0.5×0.1 cm³. Other transport parameters include detailed physics treatment and low energy cut-off at 10 keV for photons, ITS-style energy indexing and 189 keV cut-off for electrons.

Measurements

The off-axis dose profiles and the PDD curves were all generated using the Scanditronix Wellhofer water tank scanning system (Wellhofer, Germany) which consists of a 60×60×60 cm³ water tank and a three-dimensional scanning mechanism. The manufacturer's specification of repeatability of positioning the chambers with the scanning system is ±2 mm. The SLi linac was setup with gantry angle at 0° and diaphragm angle at 90° as depicted in Figure 3.6. The MCU movement controller was connected to a laptop computer with the Scanditronix Wellhofer OmniPro-Accept software for data collection. The positioning of the water tank was done by setting the tank x-axis to correspond to the linac x-size. Together with the 90° diaphragm angle, this geometry gave crossline scans in the AB direction and inline scans in the GT direction. The centre of the tank coincided with the linac central axis and with the centre of the scanning area in a horizontal plane for the central axis PDD and symmetrical profiles. Vertical height adjusted for the required focus-to-axis distance (FAD) of the scans. Scanning movements along x and y coordinates coincide with the crosswires. This was checked by moving the ion chamber along each of x and y coordinates to the limits.

The tank was filled with water for minimum depth appropriate for measurements — 10 cm below the greatest PDD measurement depth. A minimum 10 cm water margin between the nominal field size and the scanning area were also observed. The tank level was checked with a circular black levelling disc.
The ion chamber used for the scanning was an RK chamber, with an active volume of 0.12 cm\(^3\) and an inner cavity radius of 2.0 mm. The chamber position was corrected for effective point of measurement for 6 MV – it was moved 1 mm away from x-ray source. After the chamber had been positioned at the effective point of measurement, the scanning origin was set at this point. Depths (z coordinates) represented the actual measurement depths. A reference detector was positioned at the corner of the field using a holder. The high voltage for the chamber was -200 V.

**Comparisons**

ICRU Report 42 (ICRU 1987) recommends a tolerance of 2 % in dose value in the low dose gradient regions and a tolerance of 2 mm shift in isodose line in the high dose gradient regions. The generally accepted criterion for high/low dose gradient is 3 % per millimetre. The high dose gradient regions include

a. the dose build-up region where electronic equilibrium has not been established,

b. the penumbras at the field edges where there are partial shieldings by the beam modifiers and

c. regions close to inhomogeneities such that the electronic equilibrium is disturbed.

The American Association of Physicists in Medicine (AAPM, Fraass et al 1998) proposes the following tolerances for various regions (Table 3.4 and Figure 3.15):

<table>
<thead>
<tr>
<th>Type of deviation</th>
<th>Applicable region</th>
<th>Tolerance</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\delta_1)</td>
<td>on CAX beyond (d_{\text{max}})</td>
<td>2 %</td>
</tr>
<tr>
<td>(\delta_2)</td>
<td>in high dose gradient regions</td>
<td>10 % or 2 mm shift</td>
</tr>
<tr>
<td>(\delta_3)</td>
<td>beyond (d_{\text{max}}) and within the beam but not on CAX</td>
<td>3 %</td>
</tr>
<tr>
<td>(\delta_4)</td>
<td>outside the field and beyond (d_{\text{max}})</td>
<td>3 %</td>
</tr>
</tbody>
</table>

*Table 3.4 Tolerances proposed by Fraass et al (1998). \(\delta_4\) is calculated according to Equation 3.2.*
Figure 3.15 Graphical representation of different types of deviation. The solid line represents a reference curve and the dotted line is a calculated curve.

\[ \delta_1 = \frac{d(x) - d_{\text{ref}}(x)}{d_{\text{ref}}(x)} \times 100\% \]  

... 3.1

\[ \delta_3 = \frac{d(x) - d_{\text{ref}}(0)}{d_{\text{ref}}(0)} \times 100\% \]  

... 3.2

\[ \Lambda = \bar{\delta} + c \sigma \]  

... 3.3

where \( \bar{\delta} \) is the mean, \( \sigma \) is the standard deviation of \( \delta \) and \( c \) is a factor chosen by the investigator.

The concept of confidence limit assumes that the deviations at comparable locations conform to the normal distribution. This assumption is certainly not true if all regions...
Medical Linacs

are considered together simply because the high dose gradient and the out-of-field regions will skew the distribution towards the large deviation side. Venselaar and Welleweerd (2001) chose the factor \( c = 1.5 \) in Equation 3.3 arbitrarily based on experience. A larger value (> 1.5) emphasises the effect of statistical errors while a smaller value (< 1.5) emphasises that of systematic errors. It also corresponds to a 93.5 % confidence interval. The probability of real difference between two curves is 0.065 which implies that about 6.5 % of the deviations will be larger than the prescribed tolerance for that particular region. In this thesis, the factor \( c = 1.0 \) is chosen for all the comparisons to reflect the systematic error of different models. \( \Delta_{1.0} \) will be used to denote the confidence limit thus calculated.

Results and discussions

PDDs of different electron energies in a 10×10 cm² field are shown in Figure 3.16 and Figure 3.17; the comparisons are summarised in Table 3.5. The average local difference within the beam varies from 2 % (6.2 MeV) below the measured profile to 0 % (6.6 MeV), all with standard deviation about 1 %. The confidence limit changes from 3 % (6.2 MeV) to 1 % (6.5 MeV). Qualitatively, the calculated PDD approaches the measurements from below as the mean energy of the initial electron beam increases. This is as expected because the increase in electron energy results in higher bremsstrahlung energy that, in turn, gives rise to higher absorbed dose at greater depth.

Since the 6.5 MeV beam gives the smallest confidence limit, Table 3.5 suggests that this beam is of the most suitable energy. However, it must be noted that the 6.4 and 6.6 MeV beams are also within the 2 % recommended tolerance. They are still good candidates for the initial electron beam.
<table>
<thead>
<tr>
<th>Electron mean energy (MeV)</th>
<th>Mean</th>
<th>Standard deviation</th>
<th>Confidence limit (Δ₁₀)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0</td>
<td>-1 %</td>
<td>1 %</td>
<td>3 %</td>
</tr>
<tr>
<td>6.2</td>
<td>-2 %</td>
<td>1 %</td>
<td>3 %</td>
</tr>
<tr>
<td>6.4</td>
<td>-1 %</td>
<td>1 %</td>
<td>2 %</td>
</tr>
<tr>
<td>6.5</td>
<td>0 %</td>
<td>1 %</td>
<td>1 %</td>
</tr>
<tr>
<td>6.6</td>
<td>0 %</td>
<td>1 %</td>
<td>2 %</td>
</tr>
</tbody>
</table>

Table 3.5 Comparisons of PDDs in a 10x10 cm² field. Deviation between the Monte Carlo PDDs and the measurements are calculated for points beyond d_max.

Figure 3.16 Comparison of PDD at 6.5 MeV with measurements. It is the 'best' match as suggested by Table 3.5.
Figure 3.17 Comparison of various PDDs with measurements.
Further simulations are performed for all of the above initial electron beams in a 20×20 cm² field to examine the horn effect at $d_{\text{max}}$. The horn effect is caused by the over-flattening of the bremsstrahlung beam. The design of the flattening filter aims at a relatively flat dose profile at 10 cm deep in a water phantom. Because of off-axis softening of the energy spectrum caused by the flattening filter and the scattering caused by the beam modifying devices, the beam is less penetrating near its edge than at its central axis. Higher dose is therefore deposited near the beam edge at shallow depths. This is the horn effect. Its prominence gradually decreases with increased depth and it disappears completely at 10 cm deep.

Figure 3.18 shows the horn effect for different initial electron beams and they are summarised in Table 3.6. The average local difference varies between -1 % to 1 % and the standard deviations are at 1 %. The confidence limits are between 1 % and 3 %. Although the confidence limit (1 %) is the smallest for the 6.4 MeV beam, it is not clear from the average values that 6.4 MeV is the best fit. The mean value, apparently, fluctuates randomly with the electron beam energy. This apparent contradiction is resolved by examining the local differences in detail (Figure 3.19).

<table>
<thead>
<tr>
<th>electron mean energy (MeV)</th>
<th>mean</th>
<th>standard deviation</th>
<th>Confidence limit</th>
<th>slope of trend line</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0</td>
<td>0 %</td>
<td>1 %</td>
<td>2 %</td>
<td>$3.5\times10^{-3}$</td>
</tr>
<tr>
<td>6.2</td>
<td>-1 %</td>
<td>1 %</td>
<td>2 %</td>
<td>$1.7\times10^{-4}$</td>
</tr>
<tr>
<td>6.4</td>
<td>0 %</td>
<td>1 %</td>
<td>1 %</td>
<td>$3.3\times10^{-4}$</td>
</tr>
<tr>
<td>6.5</td>
<td>1 %</td>
<td>1 %</td>
<td>2 %</td>
<td>$3.9\times10^{-4}$</td>
</tr>
<tr>
<td>6.6</td>
<td>-1 %</td>
<td>1 %</td>
<td>3 %</td>
<td>$3.9\times10^{-4}$</td>
</tr>
</tbody>
</table>

Table 3.6 Comparisons of dose profiles in a 20×20 cm² field. Percentage differences between the Monte Carlo values and the measurements are calculated in the low dose gradient regions within the beam.
Figure 3.18 The horn effect of a 20×20 cm² field with different initial electron beam energies. The 6.4 MeV beam gives the best match with the measurements. The lines connecting the data points are for guiding the eye only and should not be interpreted as valid information.

Figure 3.19 Trends in local differences within the beams. This graph is the same as the sub-graph in Figure 3.18 with trend lines added. It shows that 6.4 MeV has the smallest local differences and the least dependency on off-axis distance.
Linear trend lines are fitted to the local differences in Figure 3.19. The slopes of the trend lines are listed in Table 3.6. When the mean difference and the slope are considered together, it shows that the 6.4 MeV beam has the smallest local difference and the least dependency on off-axis distance (second smallest slope in the table). Thus the mean energy of the initial electron beam is determined to be 6.4 MeV with 1 MeV fwhm. Further simulations of this initial electron beam with other fields will be shown in the following chapters, together with different phase space models for comparisons.

Studies by Lin et al (2001) and Lovelock et al (1995) have shown that the dose profile is more sensitive to the electron beam energy than the PDD curve. When the beam’s energy spread and geometry are also taken into account, Ding (2002) has shown that the dose profile is very sensitive to the beam geometry while the PDD curve depends only on energy. Similar conclusions are also derived by Sheikh-Bagheri and Rogers (2002a). They showed that the PDD curve depends only on the energy spectrum and not on the beam geometry. On the other hand, the off-axis factors are very sensitive to the electron beam geometry but not to the energy spread.

This work has shown that, for a given energy spread and beam geometry, the dose profile or the off-axis factor is more sensitive to the electron mean energy than the PDD. The dose profile is crucial to the determination of the initial electron beam parameters. The parameters determined here is compatible with those found in the literature (cf Table 3.3).

**Chapter summary**

The Elekta SLi linac treatment head is modelled with MCNPX. The PDDs and off-axis profiles of a 10×10cm² and a 20×20 cm² fields are obtained in a water tank at 100 cm SSD. Different initial electron beam parameters are simulated and the results are compared with measurements to determine which parameter set is correct. The initial electron beam is thus determined to have mean energy at 6.4 MeV with 1 MeV fwhm and 1 mm spot size.
Chapter 4  Phase Space Modelling

Although division of the linac simulation into three steps saves a significant amount of computing time, the surface source files or phase space files are usually in gigabytes which is inconvenient to handle. Many investigators have looked into ways to summarise the phase space information into compact formats. Such compact formats are known as phase space models. They offer ease of handling and, in principle, unlimited number of source particles. Some of the more notable, existing models include the point source model (Fix et al 2000, Chetty et al 2000\(^6\)), multiple source model (Ma et al 1993, Fix et al 2001a, Fix et al 2001b), virtual photon energy fluence model (Fippel et al 2003) and the correlated histogram model (Schach von Wittenau et al 1999, Hartmann Siantar et al 2001). In this chapter, the first two models are implemented. Their relative merits shall be discussed.

**Point source model**

Studies of the angular spread of the bremsstrahlung photons from a 15 MV linac show that 93.5% of the photons arrives at the isocentric plane without collision (Mohan et al 1985). It seems therefore reasonable to assume that all particles are focused at the target. This is the basic assumption in the point source model (PSM, Figure 4.1).

---

\(^6\) The model by Chetty et al (2000) is actually an improved version of the point source model and it was termed the virtual source model.
Creating the PSM

To create the PSM, the surface source file for the full Monte Carlo simulation from the previous chapter is read and the radial spatial distribution of the particles and the corresponding energy spectra are tallied in concentric rings around the central axis (Figure 4.2 to Figure 4.5). The inner-most ring is actually a disc of 2 mm in radius. Each additional ring has a 2 mm width which subtends an angle of about 0.5° at the centre of the target. The largest ring has outer radius 5.0 cm covering the projected opening of the primary collimator. The energy bins are set at 0.2 MeV intervals up to 7 MeV. Since only 0.6% of the particles in the output plane are electrons, larger bins are used for simplicity. The radial bins for electrons are 5 mm wide and the energy bins are 0.5 MeV. Alternative to a large surface source file, the model can be created from a simulation of the patient-independent components with the MCNP ring detector tallies (Chetty et al 2000) with appropriate energy bins.
Figure 4.2 Radial spatial distribution of the photons in the output plane beneath the monitor chamber.

Figure 4.3 Energy spectrum of the photons in the output plane beneath the monitor chamber. Off-axis softening of the spectrum is evident in the graph.
Figure 4.4 Radial spatial distribution of the electrons in the output plane beneath the monitor chamber.

Figure 4.5 Energy spectrum of the electrons in the output plane beneath the monitor chamber. Off-axis softening of the spectrum is evident but not as severe as for the photons.
Beam reconstruction

The radial distributions and the energy spectra (Figure 4.2 and Figure 4.3) are translated into MCNPX distributions with the $Sin$ and $SPn$ cards, and placed in the input file. Instead of using the MCNPX general source definition $SDEF$, a source subroutine was written to reconstruct the PSM beam. The source subroutine supplies all the particle parameters to the main program through some predefined global variables – position ($xxx, yyy, zzz$), direction cosines ($uuu, vvv, www$), energy (erg) and statistical weight ($wgt$). The particle position is determined by sampling the radial distribution which gives the radial position $r$ and uniform sampling of angle $\theta$ between 0 and $2\pi$:

$$xxx = r \cos \theta$$  
... 4.1

$$yyy = r \sin \theta$$  
... 4.2

and $zzz$ is a constant determined by the phase space position. Then the energy is sampled from the spectrum associated with the ring specified by $r$. Since the particles are focused at the target that sits at the origin (0, 0, 0), the direction cosines are simply the values of the normalised position vector:

$$(uuu, vvv, www) = \left(\frac{xxx, yyy, zzz}{(xxx, yyy, zzz)}\right)$$  
... 4.3

A Gaussian source biasing scheme was written into the source subroutine to increase the calculation efficiency. The radial distribution is multiplied by a Gaussian function $g(r; \mu, \sigma)$ with mean $\mu$ and standard deviation $\sigma$. The statistical weight of the particle is reduced correspondingly. $\mu$ and $\sigma$ are entered through the $RDUM$ card in the input file.

$$wgt = \frac{1}{g(r; \mu, \sigma)}$$  
... 4.4

The contaminant electrons are modelled exactly the same as the photons. The frequency of transporting an electron is sampled from the photon-electron ratio which is also entered in the input file with the $Sin$ and $SPn$ cards. The control parameters and the order of the distributions in the input file are listed in Table 4.1.
Multiple source model

The multiple source model (MSM) was first proposed by Ma et al (1993) for electron beams. It has been investigated by many authors (Deng et al 2000, Fix et al 2001a, 2001b, Chaves et al 2004) and has become the de facto standard phase space model. The central assumption in MSM is that particles from the same component share the same characteristics. This means that particles from a component can be described by an energy spectrum and a set of spatial distributions at the component and at the output plane. The flight direction is determined by the line connecting the particle position on the component plane to that on the output plane (Figure 4.6).

The MSM requires the analysis of the last interaction site of the photon before reaching the output plane. It is often used with the EGS codes because the codes provide this information. On the other hand, the MCNP(X) codes do not supply these data directly.
Figure 4.6 Multiple source model. Source particles from each component have their own spatial distribution and energy spectrum. The 'stars' in the diagram represent the last interaction sites of the particle before crossing the output plane.

Creating the MSM

In this work, the last interaction site is not obtained. To compensate for the lack of such information, the last interaction component is identified. Our phase space for each particle consists of the data of all component surfaces that it has crossed. These data include the position, direction, and energy of the particle. Since the photon crossings are recorded in a sequential order, the first crossing with energy and direction the same as those at the output plane indicates the component of last interaction. The exact interaction location is unknown but the component in which it happens can be identified. An IDL programme *McnpMSM_Decomp* was developed in-house to extract these MSM data. Figure 4.7 is the flowchart describing the algorithm.
The component sources are usually modelled by the bottom surface of the component except for the primary collimator. Since these components have symmetry around the central axis, a radial distribution is sufficient to describe a spatial distribution at the source component. A second radial distribution is needed to describe where the photons end up in the output plane. For the primary collimator,
the source is modelled with its internal conical surface. A distribution in the z-direction will suffice.

A surface source file was generated accordingly to create the phase space for MSM modelling. The simulation was essentially a repeat of the simulation in the previous chapter but with extra surface crossing recordings. Of the 1.6 million histories simulated, 1.5 million of them contribute to the output plane. A total of over 36 million tracks, about 3.3 gigabytes, were recorded because of bremsstrahlung splitting. Interactions are only identified in the target, primary collimator and the flattening filter. Figure 4.8 to Figure 4.10 are selected summaries from McnpMSM_Decomp. The relative strengths of the photon component sources are 66.5 % at target, 5.2 % at the primary collimator and 28.3 % at the flattening filter. Off-axis variation of the energy spectrum is evident in Figure 4.11 to Figure 4.13 although such variation is prominent in the flattening filter (Figure 4.13)

![Distribution of photons along z axis](image)

Figure 4.8 Results of McnpMSM_Decomp. It shows the z position of the source photons emerging from a component surface – the bottom of the target, the conical surface of the primary collimator and the bottom of the flattening filter. No photons originated from other components were recorded.
Figure 4.9 Spatial distribution of photons from the target.

Figure 4.10 Spatial distribution of the photons from the flattening filter.
Figure 4.11 Energy spectrum of photons from the target component reaching the output plane. Off-axis softening of the spectrum is very prominent.

Figure 4.12 Energy spectrum of photons from the primary collimator component reaching the output plane. Off-axis softening of the spectrum is evident but not as severe as the target.
Beam reconstruction

Reconstruction of the beam is accomplished through a source subroutine. As in the PSM, the distributions are translated into the MCNPX $Sin$ and $Spn$ cards and control parameters are passed into the source subroutine through the $IDUM$ and $RDUM$ cards (Table 4.2). The sampling for the particle position on the output plane, on the source plane for the target and the flattening filter is carried out in the manner described for the PSM. However, the sampling for the position on the primary collimator is slightly different because the source is summarised along the $z$-axis. The $x$ and $y$ positions are recovered from $r$ and a uniformly sampled $\theta$ as in Equations 4.1 and 4.2 such that $r$ is calculated according to

$$ r = t(z - zzz) $$ ...

4.5

where $t$ and $zzz$ come from the equation for the cone surface of the primary collimator,

$$ \sqrt{x^2 + y^2} - t(z - \bar{z}) = 0 $$ ...

4.6

The sampling of the energy is also analogous to the PSM. The electron sub-source is modelled as in PSM. Source biasing is not implemented.
Control parameters

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IDUM(1)</td>
<td>number of component sources, ( n )</td>
</tr>
<tr>
<td>IDUM(2)</td>
<td>number of energy spectra per component source, ( m )</td>
</tr>
<tr>
<td>IDUM(3)</td>
<td>component source starting cell</td>
</tr>
<tr>
<td>RDUM(1)</td>
<td>maximum radius of output plane</td>
</tr>
<tr>
<td>RDUM(2:n)</td>
<td>( z )-positions of component source planes</td>
</tr>
<tr>
<td>RDUM(n+1)</td>
<td>( z )-position of output plane</td>
</tr>
</tbody>
</table>

Order of distributions

1. photon-to-electron ratio
2. component source ratio
3. 1st component SOURCE spatial distribution
4. 1st component OUTPUT PLANE spatial distribution
5. 1st component energy spectrum
3+(m+2)(i-1) \( i \)-th component SOURCE spatial distribution
4+(m+2)(i-1) \( i \)-th component OUTPUT PLANE spatial distribution
5+(m+2)(i-1)+j \( i \)-th component \( j \)-th energy spectrum, \( j=0,1,2 ... \)
3+(m+2)n electron radial distribution
4+(m+2)n electron energy spectrum

Table 4.2 Control parameters and order of distributions in an MSM input file.

Results

The beams are reconstructed and transported into a water phantom at 100 cm SSD as in Chapter 3. Off-axis dose profiles and PDDs are obtained for comparison. The scoring voxels for the dose profiles have dimension 5.0×0.5×0.5 cm³ while those for the PDDs are 1.0×0.5×0.1 cm³. Results are normalised to 1 on the CAX at \( d_{\text{max}} \) and are presented in Figure 4.14 and Figure 4.17 and in Table 4.3 to Table 4.8. Also included in these figures and tables for comparisons are the results from the full Monte Carlo simulation, i.e., simulations with the original, uncompressed surface source files.
Figure 4.14 Comparisons of the PSM and FMC calculated PDDs with measurements. Local deviations are calculated according to Equation 3.1.
Figure 4.15 Comparisons of the PSM and FMC calculated off-axis dose profiles with measurements. Local deviations are calculated according to Equation 3.1.
Figure 4.16 Comparisons of the MSM and FMC calculated PDDs with measurements. Local deviations are calculated according to Equation 3.1.
Figure 4.17 Comparisons of the MSM and FMC calculated off-axis dose profiles with measurements. Local deviations are calculated according to Equation 3.1.
Qualitatively, both Figure 4.14 and Figure 4.15 show reasonable agreement between calculations and measurements. Figure 4.14 is the comparison of PDDs. The PSM calculated PDD matches well with measurements in the 5x5 cm² field but underestimates the dose after $d_{\text{max}}$ in the 20x20 cm² field. On the other hand, the MSM calculated PDDs exhibit good agreements in both fields. When the FMC results are taken into consideration, it can be seen that the FMC also show some disagreements with measurements after $d_{\text{max}}$ in the 20x20 cm² field. However, the magnitude of the PSM deviation in this region is larger than that of FMC whereas the magnitude of the MSM deviation is comparable to the FMC. It is possible that the initial electron parameters require some further tuning for large fields. Nevertheless, the MSM model is giving better PDDs than the PSM.

Comparisons of the off-axis dose profiles from both models (Figure 4.15) show good agreement between calculations and measurements inside the 5x5 cm² field and the agreement degrades in the 20x20 cm² field. Since the MSM has a better PDD, this is reflected in the profile at 10 cm deep. In fact, the MSM results are generally better than the PSM results at 10 cm deep. In the penumbra, the 5x5 cm² field shows a 1 mm shift in the calculated profiles against the measurements. The shift is within the recommended tolerance (Table 3.4). But the shift is not present in the larger field sizes. Also, the same shift is present in the FMC calculations. Even the FMC shift magnitude is the same as both PSM and MSM. Therefore, the shift is not caused by the source models. This aspect shall be pursued further in Chapter 6.

Outside the beam edge, both models show large discrepancies against the measurements. However, these deviations or discrepancies are usually expressed with respect to the dose at the CAX. The quantitative results are presented in the following sections. For data points inside the beam, the deviations are calculated according to Equation 3.1; for points outside the beam, calculations are carried out according to Equation 3.2.

**Point source model results**

Although Table 4.3 shows excellent agreement ($\Delta_{0.1} \leq 2\%$) in the dose build-up region in all fields, the PSM is poor at depths after $d_{\text{max}}$ with $2\% \leq \Delta_{1.0} \leq 5\%$. Also, the calculated PDDs are generally below the measured one with mean value of $-1\%$
in small fields and -4 % in larger fields. Contrarily, the confidence limits from the FMC are generally within the recommended tolerance.

<table>
<thead>
<tr>
<th>Field size (cm²)</th>
<th>Build-up region (δ₇)</th>
<th>After dₘₐₓ (δ₅)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>recommended tolerance 10 % mean (%)</td>
<td>s.d. (%)</td>
</tr>
<tr>
<td>5x5</td>
<td>0 (-2)</td>
<td>0 (1)</td>
</tr>
<tr>
<td>10x10</td>
<td>1 (-1)</td>
<td>1 (1)</td>
</tr>
<tr>
<td>15x15</td>
<td>0 (-1)</td>
<td>1 (1)</td>
</tr>
<tr>
<td>20x20</td>
<td>0 (-1)</td>
<td>0 (1)</td>
</tr>
</tbody>
</table>

Table 4.3 PSM deviation from measurement in the PDD. Build-up region is calculated between 0.5 cm deep and before dₘₐₓ. Values in brackets are the results of corresponding FMC simulations.

Since the normalisation is carried out at dₘₐₓ, the comparisons within the beam at this depth (Table 4.4) show acceptable tolerance Δ₁₀ = 1 % with mean value 0 % in three of the four fields and -1 % in the 20x20 cm² field. At 10 cm deep, the agreement degrades to 1% ≤ Δ₁₀ ≤ 4 % with mean value between -1 % in the 5x5 cm² field and -3 % in the 20x20 cm² field. The negative mean values also reflect the poor match between the calculated and the measured PDDs. In general, the larger the field size, the larger the disagreement. However, this is not the case with the FMC. All confidence limits from the FMC are within the recommended tolerance.

<table>
<thead>
<tr>
<th>Field size (cm²)</th>
<th>At dₘₐₓ (δ₅)</th>
<th>At 10 cm deep (δ₅)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>recommended tolerance 3 % mean (%)</td>
<td>s.d. (%)</td>
</tr>
<tr>
<td>5x5</td>
<td>0 (-1)</td>
<td>1 (1)</td>
</tr>
<tr>
<td>10x10</td>
<td>0 (-2)</td>
<td>1 (1)</td>
</tr>
<tr>
<td>15x15</td>
<td>0 (-1)</td>
<td>1 (1)</td>
</tr>
<tr>
<td>20x20</td>
<td>-1 (0)</td>
<td>1 (1)</td>
</tr>
</tbody>
</table>

Table 4.4 PSM deviation from measurements (δ₅) in the dose profiles inside the beam. Values in brackets are the results of corresponding FMC simulations.
Outside the beam (Table 4.5), similar comments apply; the larger the field size or the greater the depth, the larger the disagreement. The confidence limit at $d_{\text{max}}$ is between 1 % and 2 % with mean values generally at -1 %. At 10 cm deep, it is between 2 % and 5 % with mean value between -1 % and -3 %. The negative mean values signify that the calculation with PSM almost always underestimates the dose outside the beam. Again, the PSM confidence limits are larger than the FMC values which are within the recommended tolerance.

<table>
<thead>
<tr>
<th>Field size (cm$^2$)</th>
<th>At $d_{\text{max}}$</th>
<th>At 10 cm deep</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>recommended tolerance 3 %</td>
<td>recommended tolerance 3 %</td>
</tr>
<tr>
<td></td>
<td>mean (%)</td>
<td>s.d. (%)</td>
</tr>
<tr>
<td>5x5</td>
<td>1 (0)</td>
<td>0 (0)</td>
</tr>
<tr>
<td>10x10</td>
<td>-1 (0)</td>
<td>1 (0)</td>
</tr>
<tr>
<td>15x15</td>
<td>-1 (0)</td>
<td>1 (0)</td>
</tr>
<tr>
<td>20x20</td>
<td>-1 (-1)</td>
<td>1 (0)</td>
</tr>
</tbody>
</table>

Table 4.5 PSM deviation from measurement ($\delta$) in the dose profiles outside the beam. Values in brackets are the results of corresponding FMC simulations.

Comparing with the recommended tolerances listed in Table 3.4 (2 % on CAX beyond $d_{\text{max}}$ and 3 % otherwise), the PSM fails in the PDDs of the 15x15 cm$^2$ and the 20x20 cm$^2$ fields. Thus, it also performs unsatisfactorily at 10 cm deep. However, for confidence limits inside the beam, only the value in the 20x20 cm$^2$ field (4 %) exceeds the tolerance. Outside the beam, the confidence limits are within tolerance at $d_{\text{max}}$ but fail completely at 10 cm deep.

**Multiple source model results**

Contrary to the PSM, the MSM calculated PDD exhibits a slightly less favourable comparison to the measurements in the dose build-up region but better agreement after $d_{\text{max}}$ (Table 4.6). It underestimates the dose by 1 % (mean value) and the confidence limit is between 1 % (20x20 cm$^2$ field) and 2 % (other fields). After $d_{\text{max}}$, the confidence limit varies in the range 1 % $\leq \Delta_{1.0} \leq$ 3 %. This is much better than the PSM which has a confidence limit as large as 5 %. Also the mean values from MSM are between -2 % (20x20 cm$^2$ field) and 0 % (10x10 cm$^2$ field). They are more
consistent with measurements than the PSM which underestimates these by 1 to 4 %. Also, the confidence limits from the MSM are similar in magnitude to the FMC.

<table>
<thead>
<tr>
<th>Field size (cm²)</th>
<th>Build-up region (Θb)</th>
<th>After d_{max} (Θb)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>recommended tolerance</td>
<td>10 %</td>
</tr>
<tr>
<td>5×5</td>
<td>-1 (-2) 1 (1) 2 (3)</td>
<td>1 (2)</td>
</tr>
<tr>
<td>10×10</td>
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<td>0 (0)</td>
</tr>
<tr>
<td>15×15</td>
<td>-1 (-1) 1 (1) 2 (1)</td>
<td>-1 (-1)</td>
</tr>
<tr>
<td>20×20</td>
<td>-1 (-1) 0 (0) 1 (2)</td>
<td>-2 (-2)</td>
</tr>
</tbody>
</table>

Table 4.6 MSM deviation from measurement in the PDD. Build-up region is calculated between 0.5 cm deep and before d_{max}. Values in brackets are the results of corresponding FMC simulations.

Table 4.7 is the summary of the MSM results inside the beam. At d_{max}, the MSM shows excellent results: 2 % confidence limits with mean values between -1 % and 0 %. At 10 cm deep, it is also better than the PSM. The mean values vary from -2 % to 0 % and the confidence limits are between 1 % and 3 %. The improved mean values over the PSM reflects the better match in the MSM calculated PDDs.

<table>
<thead>
<tr>
<th>Field size (cm²)</th>
<th>At d_{max}</th>
<th>At 10 cm deep</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>recommended tolerance</td>
<td>3 %</td>
</tr>
<tr>
<td>5×5</td>
<td>-1 (-1) 1 (1) 2 (1)</td>
<td>0 (1)</td>
</tr>
<tr>
<td>10×10</td>
<td>-1 (-2) 1 (1) 2 (3)</td>
<td>-1 (-2)</td>
</tr>
<tr>
<td>15×15</td>
<td>0 (-1) 1 (1) 2 (1)</td>
<td>0 (-1)</td>
</tr>
<tr>
<td>20×20</td>
<td>0 (0) 1 (1) 1 (1)</td>
<td>-1 (-1)</td>
</tr>
</tbody>
</table>

Table 4.7 MSM deviation from measurements Θb in the dose profiles inside the beam. Values in brackets are the results of corresponding FMC simulations.

Outside the beam (Table 4.8), The MSM shows some improvements over the PSM at d_{max}. The confidence limits are between 1 % and 2 % and the mean values are between 0 % (5×5 cm² field) and -1 % (other fields). At 10 cm deep, the results are
again better than the PSM. The confidence limits vary from 1 % to 4 %. The mean values are 1 % to 3 % below the measurements.

<table>
<thead>
<tr>
<th>Field size (cm²)</th>
<th>At dmax recommended tolerance 3 %</th>
<th>At 10 cm deep recommended tolerance 3 %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mean (%)</td>
<td>s.d. (%)</td>
</tr>
<tr>
<td>5×5</td>
<td>0 (0)</td>
<td>0 (0)</td>
</tr>
<tr>
<td>10×10</td>
<td>-1 (0)</td>
<td>1 (0)</td>
</tr>
<tr>
<td>15×15</td>
<td>-1 (0)</td>
<td>1 (0)</td>
</tr>
<tr>
<td>20×20</td>
<td>-1 (-1)</td>
<td>1 (0)</td>
</tr>
</tbody>
</table>

Table 4.8 MSM deviation from measurements (Δ) in the dose profiles outside the beam. Values in brackets are the results of corresponding FMC simulations.

Comparing with the tolerances listed in Table 3.4 (2 % on CAX beyond dmax and 3 % otherwise), the MSM fails only in one case – outside the beam edge at 10 cm deep (Δ1,0 = 4 %). This is a significant improvement over the PSM.

**Discussion**

**Point source model (PSM)**

The PSM fares well for calculations inside the beam but not outside because it lacks proper modelling of the scattering in the treatment head. This conclusion is the same as Mohan *et al* (1985) and Chetty *et al* (2000). This is further supported by the analysis of the component sources in the MSM. It shows that only 66.5 % of the photons in our 6 MV beam are coming from the target reaching the output plane. This is in contrast to 93.5 % from the target reaching the isocentric plane in a 15 MV beam studied by Mohan *et al* 1985, which can be well-modelled by a point source.

For the calculations with MLC, Chetty *et al* (2000) explored the use of point source model but without explicit transport of the beam through the MLC leaves. They called their model a virtual source model. To remove the explicit transport, the authors transformed the radial distribution into a distribution in a Cartesian grid. If a
grid element is blocked by an MLC leaf, the fluence in the element is reduced to 2% to account for partial transmission through the leaf. It was found that Gaussian blurring, 2.0 to 2.5 mm fwhm depending on field size, is required to obtain good agreement with measurements near the penumbra.

The Gaussian blurring in the work by Chetty et al (2000) is needed because the penumbra is primarily caused by the secondary collimators – the jaws and the MLC leaves. PSM does not have angular spreading and therefore the penumbra is unrealistic. It also leads to the large discrepancies outside the beam edge.

**Multiple source model (MSM)**

In the MSM, the position of the particle at source is determined from \( r \) and \( \theta \) (Equation 4.1 and 4.2) where \( r \) comes from the spatial distribution at source and \( \theta \) is sampled uniformly in \([0,2\pi)\). However, the particle position in the output plane is not completely independent of the source position. For the target, this independence may be a good approximation. For other components, the particle position in the output plane is more likely to be correlated to the position in the source plane because Compton scattering is the dominant interaction and it is peaked in the forward direction (Figure 4.18). Thus, \( \theta' \), the particle position in the output plane is likely to be limited to the half ring according to \( \theta \).

![Component and Source Plane](image)

*Figure 4.18 Correlation of particle position in component plane and source plane. Since the original particle originates from the target (somewhere close to the CAX), it is more likely to end up in the blue half of the output plane than the red half after Compton scattering.*
This half-ring argument is an over-simplification but the idea was explored by Schach von Wittenau et al (1999). Thus the MSM can be improved by incorporating the directional information in the model. Their correlated histogram approach does exactly this. A series of histograms depicting the angular probabilities of the particles reaching an output plane were constructed. Sampling these histograms gave the particles’ direction, energy and weight. Then, the particle was backtracked to the base of the monitor chamber and transported downstream. This model was subsequently incorporated into the Monte Carlo dose calculation system, Peregrine, and it was shown that the calculations agreed very well with the measurements (Hartmann Siantar et al 2001).

Unfortunately, construction of the correlated histograms with MCNP(X) is difficult. This is generally true with the MSM because MCNP(X) does not supply the last interaction site directly. Unless one can rewrite the code with all the necessary tests to ensure that the rewriting does not affect the quality of the simulation, he has to rely on a large surface source file to record the particles’ emergence from each head component. As will be shown later in this section, a 3 GB surface source file may not be sufficient to provide an accurate picture of the complex interactions in the treatment head. It is likely that there are geometric or energy regions which remain undersampled.

Figure 4.19 Systematic error introduced by bin sizes. The closer the output plane is to the component source, the larger the systematic error is introduced. Thus a small bin size is necessary for an output plane close to the component source.
A further complication comes from the fact that the output plane is close to the last component. The MSM is very sensitive to the spatial bin sizes (Figure 4.19). Thus it is more common to apply the MSM to an output plane beneath the treatment head (Fix et al 2001a, 2001b) so that the direction is less prone to the error introduced by the bin size. This comes back to the problem of file size because an output plane far away means more components need to be included in the phase space.

Although the confidence limits in the $20 \times 20 \text{ cm}^2$ field are 1% and 3% at $d_{\text{max}}$ and 10 cm deep respectively (Table 4.7), some regular, ripple-like pattern can clearly be seen in the MSM dose profile in Figure 4.17. They appear in both depths and strongly suggest the presence of latent variance. To investigate the extent of this pattern, the profiles in the y-direction are also plotted over the original x-profiles (Figure 4.20) and exactly the same pattern shows up. The pattern is in fact symmetric around the CAX. This implies that the MSM was constructed from an under-sampled phase space.

![Dose Profile of 20x20 cm² field](image)

*Figure 4.20 Comparing the $20 \times 20 \text{ cm}^2$ field dose profiles in the x- and the y-directions. Relative errors in the y-profiles are of the same magnitude as in the x-profiles. They are not plotted for clarity.*
Chapter summary

Two linac source models have been implemented with MCNPX. The point source model (PSM) is simple to implement while the multiple source model (MSM) is more difficult. The difficulties arise primarily because the last interaction site is not readily supplied by the MCNP(X) code. Nevertheless, the MSM shows superior performance over the PSM simply because it accounts for the scattering properties in the various components. Thus it calculates the PDD better than the PSM; it also gives more realistic dose outside the beam edge.
Chapter 5  The Directional Spectrum Model

As shown in the previous chapter, the multiple source model (MSM) requires the details of where particles are generated. The phase space file, or the surface source file for the phase space data, must be constructed carefully to include all the necessary surfaces for the MSM analysis and for the subsequent beam reconstruction. The analysis process certainly gives some insight into the physics involved in the treatment head. However, it is natural to ask the question “what if the surface source file records the data on the output plane only?” That is, the surface source file does not have the histories of the particles; it is just a simple accumulation of particles crossing the output plane. The conventional answer is the point source model (PSM). The PSM has been shown to be inadequate in previous chapter because it assumes that particles are focused at the electron target. It would also be useful to have a model that can be constructed from a simple MCNP(X) surface source file and yet the scattering properties are well-accounted for. This work examines the energy spectrum and angular spread of the bremsstrahlung photons emerging from the ionisation chamber, in particular, their deviations from focus. An IDL interface, the MCNP(X) surface source file reader, was developed to examine this phase space information. This data driven analysis of the phase space suggests the directional spectrum model (DSM) as an alternative phase space model. The directional spectrum analysis was first presented in the Advanced Workshop on Monte Carlo Treatment Planning held in Montreal, Canada (Ma and Spyrou 2004) and a concise version of this chapter was published in the proceedings of the Monte Carlo 2005 Topical Meeting held in Chattanooga, USA (Ma et al 2005).
The Directional Spectrum Model

**MCNP(X) surface source file reader**

The MCNP(X) surface source file records the particle's data when it crosses a user specified surface. The data include particle type, energy, position \((x, y, z)\), direction cosines \((u, v, w)\), statistical weight, time and its history number. These data together constitute a particle track. To conserve storage space, the codes compress some of data into a single field so that each field is a double precision floating point number. The direction cosine \(w\) is ignored because its magnitude can be recovered from its sign and the relationship

\[ u^2 + v^2 + w^2 = 1 \quad \text{... 5.1} \]

The sign of \(w\) is incorporated into a field that records the particle type and the crossing surface. The tracks in the file are in the order they cross the surface and implicitly sorted by the history number.

To facilitate the identification of what data the file contains, a file header with the summary information is placed at the beginning of the file, before the particle tracks. The header includes the version of the code, the start and finishing time of the simulation run, number of histories and number of tracks in the file and a summary of the surfaces and cells for recording the particle tracks.

The surface source file headers from MCNP and MCNPX are different and therefore the files cannot be used interchangeably by the two codes although the tracks are of the same structure.

The MCNP(X) surface source file reader is an interface for reading both MCNP and MCNPX surface source files generated under the Unix or DOS environment (Figure 5.1). It was developed in-house and written in IDL under the Unix environment. It displays some basic information on the simulation run and those on the phase space for quick reference. The content of the surface source file header is also displayed but in the command window in which the programme is run. This arrangement provides the details, if they are needed, but without clustering the interface. It allows a choice between plotting the bremsstrahlung photon or the contaminant electron data. Assuming rotational symmetry around the central axis, various data plots can be generated on demand.
Figure 5.1 Screenshots of the MCNP(X) surface source file reader. (a) The main interface showing an energy spectrum, (b) the plot of relative errors and (c) the option menu. These figures show that the displayed spectrum is generated for energy between 0 and 7 MeV with 35 energy bins (0.2 MeV bin size) from 0 to 7 cm with 35 radial bins (0.2 cm bin size).

Figure 5.1a and b show the interface displaying the energy spectrum and its associated relative errors as functions of the off-axis or radial position. Figure 5.1c is the option menu for the user to specify the plot parameters. The menu appears
automatically when the user chooses to create a new plot and it will disappear when the user finishes with the plot settings.

Display parameters can be adjusted for closer inspection of the graph and the image can be saved in a user specified file. The display colours are optimised for on-screen display. An option is provided to save the graphs in more “printer-friendly” colours. Since not every option is applicable to all plot types, the non-applicable options are disabled and shadowed (e.g. the option for the number of particles in Figure 5.1c which is not suitable for generating energy spectra). Finally, the spectral data can be exported to a user specified text file for further processing. The MCNP(X) surface source file reader provides the following plots (Table 5.1):

<table>
<thead>
<tr>
<th>Plot type</th>
<th>Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy spectrum</td>
<td>Average over a disc, a ring or a number of rings</td>
</tr>
<tr>
<td></td>
<td>Relative errors are calculated and plotted in a separate window</td>
</tr>
<tr>
<td>Hedgehog plot</td>
<td>Vectors showing the particle energies, positions and directions in different rings</td>
</tr>
<tr>
<td></td>
<td>• original or normalised^ directions</td>
</tr>
<tr>
<td></td>
<td>• original or collapsed^ positions</td>
</tr>
<tr>
<td>Scatter plot</td>
<td>Energy vs position</td>
</tr>
<tr>
<td></td>
<td>Energy vs particle direction</td>
</tr>
<tr>
<td>Directional energy spectrum</td>
<td>Energy spectrum as a function of particle direction</td>
</tr>
</tbody>
</table>

Table 5.1 Available plot types in MCNP(X) surface source file reader. ^Explanation of these options are in the text.

Figure 5.1 is an example of a spectrum and the associated relative errors. Examples of other available plots are in Figure 5.2. Details of these plots are explained in the following sections.
Figure 5.2 Screenshots of available plots from MCNP(X) surface source file reader: (a) Hedgehog plot of particle energy, position, and direction; The particles are compressed onto the x-axis in (b) and then the directions are normalised in (c); (d) Scatter plot of energy against position; (e) Scatter plot of energy against direction and normalised direction. (f) Same as (e) but in more "printer-friendly" colours. These plots are generated with about 1,500 particles.
Energy spectrum

The calculation of the energy spectrum is an analog estimator of the “current”. It means that the particles are counted, with adjustment according to their statistical weight, as they cross the output plane. The relative error $R$ is calculated with the following equations:

$$\sigma^2 = \frac{1}{n(n-1)} \left\{ n \Sigma x_i^2 - (\Sigma x_i)^2 \right\} \quad \ldots \quad 5.2$$

and

$$R = \frac{\sigma}{\overline{x}\sqrt{n}} \quad \ldots \quad 5.3$$

where $x_i$ is the total contribution to a scoring bin by the $i^{th}$ history and $n$ is the total number of histories as discussed in Chapter 2.

Hedgehog plots

The hedgehog plot displays the particle energy, position and direction all in a single graph (Figure 5.2a). It plots the particle position $r = (x, y, z)$ within a specified ring. The direction $v$ is the unit vector $(u, v, w)$. The arrow drawn from $r$ to $r + v$ represents the particle’s position and direction. To incorporate the energy into the plot, the length of the arrow is drawn proportional to the particle energy $E$. Thus, the end point of the arrow becomes

$$r' = r + Ev \quad \ldots \quad 5.4$$

Since only the particles emerging from the ionisation chamber are recorded (no backscattered particles, cf Chapter 3 on the anti-backscatter plate), all particles in the phase space are travelling in the negative $z$-directions. Thus, the particle direction is represented by a line; the arrow head is omitted for clarity – the negative $z$-direction is implicit.
Normalisation of particle direction

The normalised direction means the particle direction with respect to the position vector. Since the point of origin is defined at focus (the electron target), the normalised direction measures the particle's deviation from focus. There are two components in the deviation: a polar angle and an azimuthal angle.

Rotational symmetry around the central axis is generally assumed (e.g. Chetty et al 2000, Liu et al 1997b, Siebers et al 1999). Siebers et al (1999) also suggest a compression technique for the phase space file by taking advantage of the symmetry. All particles at \((x, y, z)\) with direction cosines \((u, v, w)\) are rotated onto the \(x\)-axis (Figure 5.3) with the following equations:

\[
x' = r = \sqrt{x^2 + y^2} \\
y' = 0 \\
z' = z \\
u' = (ux + vy)/r \\
v' = (vx - uy)/r \\
w' = w
\]

Since \(z\) is a constant for all particles on the output plane, the particle position is represented by \(r\) alone. For \(w'\), only its sign is necessary for storage; its magnitude can be obtained from the identity equation (Equation 5.1).

Very importantly, the relative particle directions are preserved under the rotation. Compressing the particles of the same annular ring onto a single axis also enables the characterisation of the directional (angular) distribution of the particles. In particular, we examined the deviation of the flight paths from the fan line joining the electron target and the particle position in the ring. If \(r' = (x', y', z')\) and \(v' = (u', v', w')\) are the position and direction cosines obtained from Equation 5.5, the new polar angle \(\phi'\) and the new azimuthal angle \(\theta'\) are unchanged (Figure 5.3), i.e.,

\[
\begin{align*}
\phi' &= \phi \\
\theta' &= \theta
\end{align*}
\]
By normalisation, we mean a measurement with respect to the fan line. Geometrically, this normalisation is equivalent to rotating the particle direction by $\beta$ at $r'$ on the $xz$-plane so that the fan line coincides with the normal to the output plane. Since the second rotation needs to be applied to the direction cosines only, it is equivalent to a rotation around the $y$-axis:

$$s = \sqrt{r'^2 + z'^2}$$

$$u'' = (-u'z + wr)/s$$

$$v'' = v'$$

$$w'' = (-u'r - wz)/s$$

Then, the polar angle $\varphi$ and the azimuthal angle $\theta$ are simply

$$\cos \varphi = w'' \quad \tan \theta = v''/u''$$

Alternatively, $\varphi$ can be defined by the dot product of the flight direction $v'$ and the fan line $r'$:

... 5.8
In summary, the normalisation procedure involves two steps. The first step is to "collapse" all particles onto an arbitrary axis. The x-axis is chosen for convenience. The second step is to "normalise" the direction. Figure 5.2b is a hedgehog plot of the energies and directions after collapsing the particles onto the x-axis and Figure 5.2c is the same after normalisation.

**Scatter plots**

There are two types of scatter plots from the MCNP(X) surface source file reader. The first one is a simple plot of energy against position (Figure 5.2d). The second one is the energy against the normalised direction, that is, energy as a function of the polar angle and the azimuthal angle (Figure 5.2e and f).

**Directional spectrum analysis**

The directional spectrum analysis was carried out for the phase space data from a 6.4 MeV initial electron beam with 1 MeV fwhm. The beam was a uniform beam with radius 1 mm impinging perpendicularly to the electron target. It was the same beam as for the PSM and MSM in the last chapter. Five hundred million source electrons were simulated. However, bremsstrahlung splitting was not employed and all particles have the same statistical weight. The number of contaminant electrons is less likely to be under-sampled. The surface source file is 2.74 GB containing over 30.6 millions tracks.

Figure 5.4 is a series of scatter plots showing the particle energy and its flight direction over the radial distance $r$. The flight direction is expressed in the normalised azimuthal angle $\theta$ and the normalised polar angle $\varphi$ as discussed above. The plots suggest that the photons may spread evenly over $\theta$ for $r$ less than about 5cm (Figure 5.4a and b). Beyond 5cm, the photons are clustered in $\theta \leq 60^\circ$ (Figure 5.4c and d). $\theta = 0^\circ$ is on the positive x-axis and $\theta = 180^\circ$ is on the negative x-axis.
Thus, this clustering means that the photons are travelling away from the beam centre or the CAX. Figure 5.4 also shows that the photons, especially the high energy ones, are concentrated near $\phi = 0^\circ$ and there are very few photons in the region $\phi > 45^\circ$. For a field of size $20 \times 20\, \text{cm}^2$, a particle at 5 cm from the axis must have a normalised polar angle of less than $43.6^\circ$ to pass through the MLC without being attenuated. These vague observations suggest a phase space model for $r \leq 5\, \text{cm}$, $\phi \leq 45^\circ$ and uniform sampling in $\theta$.

Figure 5.4 Selected scatter plots of energy vs normalised flight direction in different rings: (a) $r < 0.2\, \text{cm}$, (b) $3.0\, \text{cm} < r < 3.2\, \text{cm}$, (c) $5.0\, \text{cm} < r < 5.2\, \text{cm}$ and (d) $6.0\, \text{cm} < r < 6.2\, \text{cm}$. $\phi$ is the normalised polar angle and $\theta$ is the normalised azimuthal angle. $\phi = 0$ is on the fan line and $\theta = 0$ is on the positive x-axis. Each plot consists of 5,000 photons.
Radial fluence

Figure 5.5a is the radial fluence distribution normalised by the area under the curve. The radial fluence increases slowly with radial distance and peaks at the radial bin between 3.5 cm and 3.6 cm. It drops off quickly between 4 cm and 5 cm. Beyond 4.8 cm, all bins have relative fluence below 0.005. Together with the fact that photons in this region are travelling in an outward direction (Figure 5.4c and d), there will be very little contribution to the beam by photons in this region. Thus, the model cut off at 5 cm is a reasonable choice.

Figure 5.5 (a) Radial fluence and angular fluence distributions for (b) small scattering angles $\phi < 0.5^\circ$, (c) medium angles $0.5^\circ < \phi < 5^\circ$ and (d) large angles $5^\circ < \phi < 45^\circ$. 
Angular fluence

The 5 cm cut-off is further supported in Figure 5.5b to d for angular fluence in \( \phi \leq 0.5^\circ \), \( 0.5^\circ < \phi \leq 5^\circ \) and \( 5^\circ < \phi \leq 45^\circ \) respectively. The angular fluence distribution remains very flat up to 4.8 cm in each \( \phi \) bin. The variation is below 1\% in almost all \( \phi \) bins. The exception is the bin \( 0.5^\circ < \phi \leq 1^\circ \) in Figure 5.5c but the variation is still below 3\%. Across the \( \phi \) bins, the angular fluence peaks at the bin \( 0.1^\circ < \phi \leq 0.2^\circ \) and falls off rapidly before reaching \( \phi = 1^\circ \) (Figure 5.5a). Beyond \( 1^\circ \), the angular fluence is very much a constant (Figure 5.5c and d). In fact, photons within \( 0.5^\circ \) account for 72\% of the total number of particles within 5 cm from the CAX.

Beyond 5 cm, the angular fluence varies dramatically both in \( r \) and in \( \phi \). In general, it increases with \( \phi \) (Figure 5.5b–d). For small angles \(( \phi \leq 0.5^\circ \), Figure 5.5b\), it decreases as \( r \) increases. However, there is no clear pattern for larger angles (Figure 5.5c and d). This lack of pattern is the result of the photons being highly scattered and therefore they are low in energy as well (Figure 5.4c and d).

Directional energy spectra

The plots of \( d\Phi/dE \) across \( \theta \) (Figure 5.6) also suggest that \( d\Phi/dE \) is approximately independent of \( \theta \) for \( \phi \leq 0.5^\circ \). This independence is true at the CAX due to the rotational symmetry around the axis, but it degenerates as \( \theta \) increases or as \( r \) increases (Figure 5.6b and c). Since the particles are predominantly in the small \( \phi \) region, the total directional energy spectrum over \( \theta \), \( d\Phi'(E,\phi,r)/dE \), is a reasonable representation of \( d\Phi(E,\phi,\theta,r)/dE \):

\[
\frac{d}{dE} \phi'(E,\phi,r) = \int_\phi \frac{d}{dE} \phi(E,\phi,\theta,r) \, d\theta
\]  

... 5.10

Figure 5.6d shows the resulting directional energy spectra.
Figure 5.6 Selected directional energy spectra for the ring $3.0 \text{ cm} < r < 3.5 \text{ cm}$.

**Directional spectrum model**

The directional spectrum model (DSM) is the result of the analysis described above. It assumes that the directional energy spectrum, which is a function of energy, off-axis position and angular deviation from focus, represents the original phase space data (Figure 5.7).
Creating the DSM

The model can be generated by the IDL programme above or alternatively, be obtained with a tallyx subroutine. The subroutine is also helpful in checking the correctness of the source implementation. It works in conjunction with

1. a type 1 surface current tally,
2. a tally segment (FSn) card that sets up the radial bins, a tallyx input (FUN) card that sets up the cosine bins and
3. a tally energy (En) card that sets up the energy bins.

The type 1 surface current tally by itself gives the total number of particles crossing a plane. The FSn and the En cards divide the tally into bins in the usual MCNP/MCNPX manner. The FUN card was chosen over the usual tally cosine (Cn) card because the Cn card works with a single reference vector but our reference vector (the fan line) depends on the particle position. Thus, our tallyx subroutine examines the particle's radial position on the output plane, its energy and its direction of crossing with respect to the fan line according to Equations 5.9 and 5.10.
The appropriate bin of the tally will then be credited with a particle. The distributions generated under DSM include:

1. a radial fluence distribution describing the number of particles in the 25 rings or radial bins (0 cm ≤ r ≤ 5 cm, 0.2 cm bin size),

2. twenty five angular fluence distributions (0° ≤ θ ≤ 45°, 0.1° bin size at small θ values and variable bin sizes at larger ones, 13 bins in total) associated with each of the 25 radial bins, describing the number of particles per unit scattering angle with respect to the fan lines and

3. three hundred and twenty five energy spectra (0 MeV ≤ E ≤ 7 MeV, 0.2 MeV bin size) for each combination of the 25 radial bins and 13 scattering angle bins.

**Beam reconstruction**

As in the PSM and MSM, all distributions are translated into the MCNP/MCNPX $SIn$ and $SPn$ card format and incorporated into the simulation input file. The control parameters are passed from the input file into source through the $IDUM$ and the $RDUM$ cards. The Gaussian source biasing and an electron sub-source as in PSM are also implemented. Table 4.2 lists out the control parameters and the distributions required by the source subroutine.

The source subroutine is essentially the reverse process of the tallyx subroutine. A particle is first sampled for its radial position which will subsequently be converted into Cartesian coordinates with the assumption of symmetry around the CAX. The appropriate angular fluence distribution is then sampled for the flight direction. Finally, the energy spectrum corresponding to the particle’s radial position and its flight direction is sampled for the particle energy.
### Control parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IDUM(1)</td>
<td>source starting cell</td>
</tr>
<tr>
<td>IDUM(2)</td>
<td>number of photon radial bins, ( n )</td>
</tr>
<tr>
<td>IDUM(3)</td>
<td>number of photon polar angle bins, ( m )</td>
</tr>
<tr>
<td>IDUM(4)</td>
<td>number of electron radial bins, ( k )</td>
</tr>
<tr>
<td>RDUM(1)</td>
<td>( z )-position of output plane</td>
</tr>
<tr>
<td>RDUM(2)</td>
<td>( \mu ), the mean of the Gaussian radial position biasing</td>
</tr>
<tr>
<td>RDUM(3)</td>
<td>( \sigma ), the standard deviation of the biasing</td>
</tr>
</tbody>
</table>

### Order of distributions

1. photon-to-electron ratio
2. photon radial distribution (Gaussian biased)
3. photon angular distribution
4. photon energy spectra
5. electron radial distribution (Gaussian biased)
6. electron energy spectra

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>photon-to-electron ratio</td>
</tr>
<tr>
<td>2</td>
<td>photon radial distribution (Gaussian biased)</td>
</tr>
<tr>
<td>3</td>
<td>photon angular distribution</td>
</tr>
<tr>
<td>4</td>
<td>photon energy spectra</td>
</tr>
<tr>
<td>5</td>
<td>electron radial distribution (Gaussian biased)</td>
</tr>
<tr>
<td>6</td>
<td>electron energy spectra</td>
</tr>
</tbody>
</table>

**Table 5.2** Control parameters and order of distributions in an DSM input file.

The subroutine *source* reconstructs the photon beam in the following steps:

1. Assign type 'photon', weight '1' and starting time '0' to the particle.
2. Sample the radial fluence distribution for the ring \( r \) on the output plane to determine the starting position of the particle.
3. Sample the angular fluence distribution associated with the ring \( r \) for the normalised polar angle \( \varphi \).
4. Sample uniformly for the normalised azimuthal angle. Together with \( \varphi \), the direction cosines relative to the normalised fan line was determined.
5. Perform an inverse transformation of the Equations 5.7 and 5.8 on the direction cosines for the actual flight direction.
6. Sample the appropriate directional energy spectrum according to the normalised scattering angle \( \varphi \) and the ring \( r \) for the particle energy.
In step 4, we used the MCNPX built-in subroutine *rotas* to sample the normalised azimuthal angle uniformly. The actual function of *rotas* is to sample the direction cosines of a vector uniformly on the surface of a cone such that the tail of the vector is always the cone vertex. The cone is specified by a reference vector, which is the cone axis, and the cone angle between the surface and the reference vector. By setting the normalised fan line as the reference vector, setting the normalised scattering angle as the cone angle and letting *rotas* to determine the direction cosines for a particle, steps 4 and 5 were combined into a single step. The inverse transformation was implicitly taken care of. This also illustrates that the normalised flight angles can be defined without the second rotation.

To increase the computation efficiency, we had written into the source subroutine a variance reduction technique of Gaussian source position biasing. The radial fluence probability distribution is multiplied by a Gaussian probability density function with a mean equal to the radial position of the field centre and a full width half maximum equal to four to eight times the field size back-projected onto the phase space plane. The particle weight was adjusted by the inverse of the Gaussian probability density function. The factor was chosen so that the Gaussian function would not decrease to zero too rapidly and the radial position sampling was not over-biased.

**Results**

The beams are reconstructed and transported into a water phantom at 100 cm SSD as in Chapter 3. Off-axis dose profiles and PDDs are obtained for comparison. In the $5 \times 5$ cm$^2$ field, the scoring voxels are $0.2 \times 1.0 \times 0.5$ cm$^3$ for the dose profiles and $0.2 \times 0.2 \times 0.1$ cm$^3$ for the PDD. In the larger fields, they have dimension $5.0 \times 0.5 \times 0.5$ cm$^3$ and $1.0 \times 0.5 \times 0.1$ cm$^3$ for the dose profiles and the PDDs respectively. Results are normalised to 1 on the CAX at $d_{\text{max}}$. They are presented in Figure 5.8 and Figure 5.9 and in Table 5.3 to Table 5.5. Also included in these figures and tables for comparison are the results from the full Monte Carlo simulation (FMC), i.e., simulations with the original, uncompressed surface source files.
Figure 5.8 Comparisons of the DSM and FMC calculated PDDs with measurements. Local deviations are calculated according to Equation 3.1.
Figure 5.9 Comparisons of the DSM and FMC calculated off-axis dose profiles with measurements. Local deviations are calculated according to Equation 3.1.
Qualitatively, Figure 5.8 shows that the PDD from the DSM slightly over-estimates dose in the 5×5 cm\(^2\) field and the discrepancy increases with depth. This discrepancy is small as its maximum is about 5%. On the other hand, the discrepancies from the FMC results for the same field show a much lesser dependency on depth. The deviation from measurement is more severe in the larger field (20×20 cm\(^2\)). The DSM under-estimates the dose throughout the range after \(d_{\text{max}}\), particularly between 5 cm and 20 cm deep. Similar but less severe trend is also observed in the FMC results.

In the off-axis dose profile comparisons (Figure 5.9), the DSM improvements over the other two models are obvious in two depths and in both field sizes. The DSM profiles follow closely with the measurements. Most notable is that the DSM gives very good agreement with measurements outside the field. This is in stark contrast to the two models (PSM and MSM) discussed in the previous chapter. As noted in the last chapter, there is a shift in the 5×5 cm\(^2\) profiles. The DSM profiles show similar characteristics as the FMC profiles. The mismatches in the PDDs are also reflected in the off-axis profiles; the 5×5 cm\(^2\) profile at 10 cm deep is generally above the measurement whereas the 20×20 cm\(^2\) profile at the same depth is generally beneath the measurements.

Quantitative results are summarised in Table 5.3 to Table 5.5. Table 5.3 is the comparisons on the PDDs. For the 5×5 to 15×15 cm\(^2\) fields, the confidence limits from the DSM are similar to those from the FMC, meaning that the DSM is a good representation of the original phase space. Also, the confidence limits are in the range \(1\% \leq \Delta_{1,0} \leq 3\%\) within the recommended tolerance.
The Directional Spectrum Model

<table>
<thead>
<tr>
<th>Field size (cm²)</th>
<th>Build-up region (Δ₀) recommended tolerance 10%</th>
<th>After d_max (Δ₀) recommended tolerance 2%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mean (%) s.d. (%) Δ₁₂₀ (%)</td>
<td>mean (%) s.d. (%) Δ₁₂₀ (%)</td>
</tr>
<tr>
<td>5x5</td>
<td>-2 (-2) 1 (1) 3 (3)</td>
<td>2 (2) 1 (1) 3 (3)</td>
</tr>
<tr>
<td>10x10</td>
<td>1 (-1) 1 (1) 2 (2)</td>
<td>2 (0) 1 (1) 3 (2)</td>
</tr>
<tr>
<td>15x15</td>
<td>0 (-1) 1 (1) 1 (1)</td>
<td>0 (-1) 1 (0) 1 (1)</td>
</tr>
<tr>
<td>20x20</td>
<td>2 (-1) 1 (1) 3 (2)</td>
<td>-3 (-2) 1 (1) 4 (3)</td>
</tr>
</tbody>
</table>

Table 5.3 DSM deviation from measurement in the PDD. Build-up region is calculated between 0.5 cm deep and before d_max. Values in brackets are the results of corresponding FMC simulations.

As in the PSM, MSM and FMC calculations, normalisations are carried out at d_max.

The confidence limits are expected to behave well inside the beam at this depth. Table 5.4 shows that the DSM confidence limits are comparable to those from the FMC and more importantly, comparable both at d_max and at 10 cm deep. Again as in the PDDs, all fields other than the 20x20 cm² field have confidence limits within tolerance. Even so, the 20x20 cm² confidence limits (3%) are just larger than the tolerance. Similar results are also observed outside the beam (Table 5.4); only the 20x20 cm² confidence limits (3%) are larger than the tolerance. These results are much better than those obtained with PSM and MSM, especially for the results outside the beam edge.

<table>
<thead>
<tr>
<th>Field size (cm²)</th>
<th>At d_max recommended tolerance 3%</th>
<th>At 10 cm deep recommended tolerance 3%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mean (%) s.d. (%) Δ₁₂₀ (%)</td>
<td>mean (%) s.d. (%) Δ₁₂₀ (%)</td>
</tr>
<tr>
<td>5x5</td>
<td>0 (-1) 1 (1) 1 (1)</td>
<td>2 (1) 0 (1) 2 (1)</td>
</tr>
<tr>
<td>10x10</td>
<td>-1 (-2) 1 (1) 2 (3)</td>
<td>-1 (-2) 1 (1) 1 (2)</td>
</tr>
<tr>
<td>15x15</td>
<td>0 (-1) 1 (1) 1 (1)</td>
<td>-1 (-1) 1 (1) 1 (2)</td>
</tr>
<tr>
<td>20x20</td>
<td>-1 (0) 2 (1) 3 (1)</td>
<td>-2 (-1) 1 (1) 3 (2)</td>
</tr>
</tbody>
</table>

Table 5.4 DSM deviation from measurements (Δ₀) in the dose profiles inside the beam. Values in brackets are the results of corresponding FMC simulations.
The Directional Spectrum Model

<table>
<thead>
<tr>
<th>Field size (cm²)</th>
<th>At dₑ₀ recommended tolerance 3 %</th>
<th>At 10 cm deep recommended tolerance 3 %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mean (%)</td>
<td>s.d. (%)</td>
</tr>
<tr>
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<td>0 (0)</td>
<td>0 (0)</td>
</tr>
<tr>
<td>10x10</td>
<td>0 (0)</td>
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</tr>
<tr>
<td>15x15</td>
<td>0 (0)</td>
<td>0 (0)</td>
</tr>
<tr>
<td>20x20</td>
<td>0 (-1)</td>
<td>0 (0)</td>
</tr>
</tbody>
</table>

Table 5.5 DSM deviation from measurement (Δₑ₀) in the dose profiles outside the beam. Values in brackets are the results of corresponding FMC simulations.

Discussion

The DSM assumes a uniform particle distribution in the azimuthal angles. This is certainly true at the CAX simply because of the rotational symmetry around it. At CAX, the assumption holds true for all polar angles, that is, uniform particle distribution in the azimuthal angle regardless the deviation from focus. At a ‘small’ distance from the CAX, this uniformity still holds at ‘small’ polar angles. However, the uniformity degrades with increase in polar angle and with increase in off-axis distance. Such degradation in the uniformity assumption is clearly shown in Figure 5.6. The figure is a plot of the directional energy spectra for the ring 3.0 cm < r < 3.5 cm. At small angles (less than 5°, Figure 5.6a), the assumption is reasonable although a clear degradation is evident. At large angles (larger than 5°, Figure 5.6b and c), it is clear that the particles are concentrated in the middle, i.e., in the outward directions. Hence there should be more particles going away from the CAX than towards the CAX. The uniformity assumption forces as many particles going towards the CAX as there are going away from it. This breakdown of the uniformity assumption continues as the off-axis distance increases. At distances larger than 5 cm, the assumption breaks down completely. This is evident from Figure 5.4c and d as mentioned in the section on the directional spectrum analysis.

However, this breakdown is not a problem for small field sizes because the ‘wrong’ particles are mostly blocked by the beam shaping devices. For larger field sizes, these particles are no longer blocked and they might contribute to the dose in the phantom or patient resulting in the introduction of a systematic error into the calculation. The magnitude of this systematic error depends on the relative
abundance of the above-mentioned extraneous photons. Figure 5.5b to d show that photons at angles larger than 0.5° account for about 8% of the total within 5 cm radius (photons beyond 5 cm are not modelled in the DSM). Combined with the fact that the extraneous photons arise mostly in the outer rings and they are in the outward directions, the contribution of these photons to the dose should be reasonably small. Since the measurements for the maximum 40×40 cm² field are not available, a less vigorous comparison was made between the FMC and the DSM calculated dose distribution (Figure 5.10). The relative errors are less than 5% in general and not plotted for clarity and simplicity.

In fact, a very good match was obtained between the DSM and FMC calculated dose profiles in the largest possible field, 40×40 cm². The match at 10 cm deep is as good as the match at $d_{\text{max}}$. This implies that the DSM calculated PDD will match with the FMC calculated one in the largest possible field. There is no shift at the beam penumbras. Therefore, it can be concluded that the DSM does not introduce observable systematic error to the original phase space. Since the DSM models very
well the scattering properties within the linac head, the results inside and outside the beam agree excellently with measurements.

**Chapter summary**

We have presented a new phase space modelling technique that we termed the directional spectrum model. Very good agreements, in terms of off-axis dose profiles and percentage depth dose curves, have been obtained in the comparisons with measurements from 5×5 cm² field to 20×20 cm² field. Calculations in the 20×20 cm² field with the FMC and the DSM also agree well in terms of dose profiles at different depths. Thus the directional spectrum model represents the original phase space data accurately. Furthermore, the model directly couples the energy spectrum to the position and flight direction of the particles. This is a novel technique for examining the phase space data. Further studies of its performance in different fields should be carried out.
Chapter 6 Application of DSM to Intensity Modulated Radiotherapy

Introduction

As already mentioned in Chapter 1, each beam portal in conventional conformal radiotherapy is shaped to the cross-sectional contour of the tumour presented to the beam’s eye view. In contrast, each beam portal in intensity modulated radiotherapy (IMRT) creates a radiation field conformal to the three-dimensional profile of the tumour in addition to the cross-sectional contour (Figure 6.1). During the delivery of each IMRT beam, the MLC leaves are re-configured many times in step-and-shoot mode or continuously in dynamic mode. Thus each portal is composed of many on-axis and off-axis small fields, as well as many irregularly shaped fields.

Since IMRT delivers radiation fields conforming tightly to the tumour, it allows higher dose to be administered to the tumour. Dose escalation treats the cancer more efficiently than conventional methods (Pirzkall et al 2000). The efficacy of IMRT is still a controversial topic because of the increased dose to normal tissue arising from

Figure 6.1 Concept of IMRT (Webb 1997). Two beam portals are illustrated in this drawing.
the scattered photons (Lillicrap et al 2000, Williams and Hounsell 2001). The corrections applied to the superposition/convolution dose calculation engines are complex and often found to be insufficient. Monte Carlo calculations are, therefore, an attractive alternative (Laub et al 2000, Ma et al 2000). In this chapter, the potential of applying the directional spectrum model (DSM) to IMRT will be tested and assessed against measurements.

Statistical fluctuation is an integral part of any Monte Carlo calculation. Very long simulations can, in principle, render the fluctuation negligible. Unfortunately, it is not always possible to carry out these long simulations. As discussed in previous chapters, there are many factors limiting the length of a simulation. Long simulations are certainly unfeasible in clinical applications. Several authors have been exploring the use of digital filters to remove the statistical noise in the dose distributions (Deasy 2000, Deasy et al 2001, Fippel and Nüsslin 2003, Miao et al 2003). Others attempts to remove the noise in the dose volume histograms (Jiang et al 2000, Sempau and Bielajew 2000). Kawrakow (2002) argues that such denoising techniques constitute the ‘last’ variance reduction technique available to the Monte Carlo method and they are particularly suitable for the initial trial and error phase in treatment planning calculations.

**Principles of Denoising**

Digital filters are used extensively in imaging enhancements. One of the enhancements is smoothing for noise reduction which can be achieved in frequency domain or spatial domain. A frequency domain filter operates on the Fourier transform of the image and removes unwanted frequency components. Since noise gives rise to the high frequency component, a low-pass filter can reduce the noise level. The Fourier transform of a Gaussian function is still Gaussian. The high frequency components are removed very effectively.

A spatial filter operates on individual pixels by summing the weighted pixel values in its neighbourhood:

\[ g(x,y) = \sum_i \sum_j w(x_i, y_j) f(x_i, y_j) \]

... 6.1
where \( w(x, y) \) specifies the spatial mask; \( f(x, y) \) and \( g(x, y) \) are the original and the enhanced image respectively.

It was shown by Sempau and Bielajew (2000) that the variance of the dose deposition in a scoring voxel is proportional to the dose deposited per history:

\[
\sigma^2(d) = C \frac{d}{N} \quad \text{... 6.2}
\]

where \( d \) is the average dose deposition in a voxel, \( N \) is the number of histories and \( C \) is the proportionality constant. From the central limit theorem, the average dose deposition, \( d \), conforms to a Gaussian distribution as discussed in Chapter 2.

Buades et al (2005a) defines the noise seen by the denoising method as method noise. It is the difference between the noisy image and the denoised image. In this study, it is the difference between the Monte Carlo calculated dose distribution and the denoised distribution:

\[
n(x, y) = f(x, y) - g(x, y) \quad \text{... 6.3}
\]

where \( n(x, y) \) is the method noise, \( f(x, y) \) and \( g(x, y) \) are the Monte Carlo calculated dose distribution and the denoised distribution respectively. Ideally, the method noise looks exactly like white noise, without any structure. The root mean square (RMS) of method noise is often used as a measurement of the performance of the filter.

\[
RMS = \sqrt{\frac{1}{M} \sum_i \sum_j n(x_i, y_j)^2} \quad \text{... 6.4}
\]

where \( M \) is the number of pixels in the image. Two simple denoising schemes are explored in this study. The first denoising scheme uses a Gaussian filter and the second one uses a median filter. With Gaussian filter, the mask \( w(x, y) \) in Equation 6.1 is a Gaussian function of zero mean and standard deviation \( \sigma \). With a median filter, \( w(x, y) \) returns the median of the neighbourhood of \((x, y)\).
**Materials and methods**

The fields studied in the previous chapters are primarily shaped by the x- and y-diaphragms. The effects from the MLC are less significant. The irregular fields in this chapter are shaped primarily by the MLC leaves. They are designed to assess the DSM performance with the MLC, in particular, the shape of the penumbra.

![3D dose profile under 1 MLC leaf](image)

*Figure 6.2 Dose distribution under a single MLC leaf in a 20×20 cm² field. The effect of the leaf tip extends from y = -0.5 cm to y = 1.5 cm.*

Figure 6.2 is the dose distribution under a single MLC leaf. The leaf was set at the CAX plane (AB = 0 cm) and the rest of the leaves and the diaphragms were set accordingly for a 20×20 cm² field. The distribution was obtained from a simulation with the original phase space data. It shows clearly that the effect of the leaf tip extends to about 1.5 cm only from the CAX. Beyond 1.5 cm, the dose distributes...

---

7 Refer to Figure 3.6 for the orientation of the MLC leaves with respect to the definitions of AB and GT directions.
evenly along the length of the leaf. Thus, a scoring voxel can be several centimetres long in the AB direction without affecting the validity of the profile across the leaf in the GT direction provided that the voxel size in the GT direction is small with respect to the dose gradient.

**MLC penumbrae**

An irregularly shaped field as shown in Figure 6.3 is used for checking the MLC penumbrae. Five leaves from each bank are extended into a $30 \times 36 \text{ cm}^2$ field set by the x- and y-diaphragms. Measurements are made at $d_{\text{max}}$ across the leaves at 7.5 cm from the CAX plane on both sides. The water phantom is located at 100 cm SSD and the detector is an RK chamber. Since the leaves have various lengths inside the field, the measurements include leaf profiles close to the leaf tip and also profiles that come from the leaf body. A major difference between the two measurement locations is that the leaves are evenly spaced at 7.5 cm while the other one at -7.5 cm has varying spacing among the leaves.

![MLC Settings](image)

*Figure 6.3 Irregular $30 \times 36 \text{ cm}^2$ MLC field. Colour lines indicate the approximate position of the x- and y-diaphragms. The dotted lines mark the measurement and Monte Carlo tally positions at 7.5 and -7.5 cm from the CAX plane. The horizontal and vertical directions in the diagram correspond to the AB and GT directions respectively.*
The Monte Carlo simulation transports the DSM beam into the water phantom as in the measurement configuration. Since the leaves are set at 5 cm from the CAX plane, the scoring voxel dimension along the length of the leaf is chosen to be 1 cm to avoid being affected by the leaf tips. Therefore, the scoring voxels have dimensions 0.2 cm in the GT direction (scanning direction), 1.0 cm in the AB direction (along the length of the leaves) and 0.5 cm centred at $d_{\text{max}}$.

**Diamond-shaped field**

Although other comparisons in this thesis provide a considerable amount of data about the penumbra in various field sizes, these data are generated under a relatively simple condition, namely, the penumbra formed by a single leaf. This exercise is designed to assess the shift in isodose lines under more realistic conditions. The test field is a diamond-shaped field formed by the MLC leaves (Figure 6.4).

![MLC Settings](image)

**Figure 6.4 Diamond-shaped MLC field. Colour lines indicate the approximate position of the x- and y-diaphragms. The horizontal and vertical directions in the diagram correspond to the AB and GT directions respectively.**

Measurements were made with Kodak EDR film in a solid water phantom. The phantom measured $20 \times 20 \times 17$ cm$^3$ and the film was sandwiched between the solid
water slabs at a depth of 9 cm. The SSD was 94 cm. Thus the film was located at 103 cm from the electron target. It was exposed to 50 cGy of photon dose and was read by the Scanditronix RFA-300 film densitometer which was calibrated for automatic generation of the isodose lines for comparison.

The Monte Carlo simulation was carried out under the same conditions as with the experiment except for the phantom material. Since the exact elemental composition of solid water is unknown, liquid water was used in the simulation. Also the presence of the film is ignored in the simulation. There were 10,000 scoring voxels, 0.1×0.1×0.5 cm³ each, covering an area of 10×10 cm².

To obtain the isodose curves from the DSM calculated dose distribution, the distribution is first normalised to 1 not at the CAX but at the average dose within the field. This normalisation procedure is to alleviate some problems caused by the statistical fluctuation within the field. The curves are then generated from the normalised distribution with the IDL contour function. To measure the shift in the isodose curves, both sets of isodose curves – the film measurements and the DSM calculations – are plotted in the same graph which is subsequently converted into an image. Between 30 and 40 points on each curve are selected for measurements based on their identifiability in the image. These points include those on the x- and y-axis and the corners formed by the MLC leaves. The distance between two points in the image is measured using another IDL function measure developed in-house (Figure 6.5). Since the landmark features in the curves are not always clear or identifiable, some degrees of subjective judgement are necessary in choosing the measurement points. Nevertheless, quantitative estimates can still be obtained with this approach. Relative merits of this approach will be discussed further in later sections.

To maintain the correct sign of the shift in each measurement, a point on the reference curve must be chosen first and the corresponding point on the other curve second. In this work, the isodose curves from the film are the reference curves. The shift in the calculated curve with respect to the reference is positive if the shift happens to be away from the origin (CAX). Conversely, the shift is deemed to be negative.
The measurements are labelled with thick black lines for identification (Figure 6.5). They are displayed in column D in the measurement table on the right hand side of the interface. The endpoints of the lines are also listed in the table, which can be revealed by moving the scrolling bar to the right. Underneath the table is the statistical summary showing the number of measurements, the mean and the standard deviation. Both the labelled graph and the measurement data can be saved in files for record.

Figure 6.5 IDL function measure for measuring the isodose shifts. The thick black lines, highlighted here in red circles, label the measurement positions. Note that some lines are too short to be labelled properly but the details are always available in the measurement table on the right.

Results

MLC penumbras

Figure 6.6 and Figure 6.7 are the results of the simulation compared with measurements. Because of the relatively small spacing between the MLC leaves, the field is analogous to a series of small fields situated close to each other. The widths
of the leaf shadows, or the widths of the open beam regions, from calculation agree very well with the measurements in both figures. However, the calculated profiles have sharper penumbras at every leaf edge. This observation is consistent with other studies on the RK chamber performance in measuring the penumbras, e.g., Metcalfe et al (1993) and Bucciolini et al (2003).

The profile in Figure 6.6 shows that the calculations in the open beam regions roughly follow the measurements because of the statistical fluctuations. However, the calculation in the leaf shadows has much lower dose than measurements. In general, the calculated values are only 50% of the measured ones near the centre of the leaf umbrae, i.e., at the points of local minima. Similarly, the calculated dosages at the field edges are also lower than the measured ones.

Figure 6.6 Dose profile across the MLC field at 7.5 cm from the CAX plane. Lines are drawn between points for guiding the eye. The calculated dose near the centre of a leaf umbra (in red circle) is about 50% of the measured value.
Similar comments are also applicable to Figure 6.7 showing the profile at -7.5 cm. However, the open beam regions at 15 and -15 cm show large differences between calculations and measurements. At 15 cm, the calculated dose is about 28% higher than the measured one. At -15 cm, the difference increases to 30%. It is also interesting to note that the measured profiles at these two locations have a large difference in relative dose, about 15%, although both are generated by opening a single leaf. On the other hand, the difference in the calculated values at these locations are less pronounced, about 3% only.

![MLC profile at -7.5 cm](image)

*Figure 6.7 Dose profile across the MLC field at -7.5 cm from the CAX plane. Lines are drawn between points for guiding the eye. The calculated dose near the centre of a leaf umbra (in red circle) is about 50% of the measured value.*

**Diamond-shaped field**

The simulation results from the diamond field are plotted in Figure 6.8 which shows (a) the dose distribution normalised by the number of simulation histories and (b) the relative errors. Within the field, the relative errors are less than 5%. Outside the field, the relative error grows very quickly with the off-axis position because of insufficient number of particles.
Figure 6.8 Dose distribution calculated by DSM in the diamond-shaped field.
The dose distribution is renormalized to 1 at CAX to give relative doses for comparison with the film measurements. The resulting isodose curves at 0.2, 0.5, 0.8 and 0.95 of the dose at CAX are presented in Figure 6.9. The agreement between the DSM calculations and measurements are reasonably good at 0.2, 0.5 and 0.8 levels. At 0.95 level, the statistical fluctuation in the DSM calculation makes the comparison difficult although it can be seen from the figure that the calculated isodose curve generally wriggle along the measurements. Quantitative estimates of the shifts are presented in Table 6.1. The mean shift in each isodose curve is less than 1 mm with standard deviation about 0.5 mm. The confidence limits ($\Delta_{1.0}$) are between 1.3 and 1.5 mm which are well within the recommended tolerance of 2 mm.

![Isodose curves of the diamond shape field](image)

*Figure 6.9 Comparison of isodose curves from DSM calculation in water, without denoising, and film measurement in solid water. Solid lines are the measured isodose curves and dotted lines are the Monte Carlo calculated ones. Different colours represent the isodose levels.*
Table 6.1 Shift in the isodose curves in the raw DSM calculated data in the diamond-shape field as measured from Figure 6.9.

<table>
<thead>
<tr>
<th>Isodose</th>
<th>mean (mm)</th>
<th>s.d. (mm)</th>
<th>$\Delta_{1.0}$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.95</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>0.8</td>
<td>1.0</td>
<td>0.5</td>
<td>1.5</td>
</tr>
<tr>
<td>0.5</td>
<td>0.8</td>
<td>0.6</td>
<td>1.4</td>
</tr>
<tr>
<td>0.2</td>
<td>0.8</td>
<td>0.5</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Table 6.2 Shift in the isodose curves in the Gaussian-filter denoised DSM calculated data in the diamond-shape field as measured from Figure 6.10.

<table>
<thead>
<tr>
<th>Isodose</th>
<th>mean (mm)</th>
<th>s.d. (mm)</th>
<th>$\Delta_{1.0}$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.95</td>
<td>0.0</td>
<td>0.9</td>
<td>0.9</td>
</tr>
<tr>
<td>0.8</td>
<td>0.8</td>
<td>0.4</td>
<td>1.2</td>
</tr>
<tr>
<td>0.5</td>
<td>1.0</td>
<td>0.4</td>
<td>1.4</td>
</tr>
<tr>
<td>0.2</td>
<td>1.2</td>
<td>0.4</td>
<td>1.6</td>
</tr>
</tbody>
</table>

The results from the DSM calculations, denoised with the Gaussian filter, are presented in Figure 6.10 and Table 6.2. Figure 6.10 shows that the 0.95 level isodose curves after denoising follows the measurements much better than that of raw calculation data as in Figure 6.9. The other isodose curves also show smoother appearance than in Figure 6.9. Furthermore, all of the 0.95 level curves inside the field are removed. Therefore, quantitative comparison of this level can be made. Table 6.2 shows that the mean shift in the 0.95 level curve is 0.0 mm with 0.9 mm standard deviation. The confidence limit is 0.9 mm. For the other curves, the mean shifts are between 0.8 and 1.2 mm, all with 0.4 mm standard deviation. The confidence limits ($\Delta_{1.0}$) are between 1.2 and 1.6 mm, within the recommended tolerance of 2 mm.
Figure 6.10 Comparison of isodose curves from DSM calculation in water, Gaussian denoised, and film measurement in solid water. Solid lines are the measured isodose curves and dotted lines are the Monte Carlo calculated ones. Different colours represent the isodose levels.

Figure 6.11 Comparison of isodose curves from DSM calculation in water, median denoised, and film measurement in solid water. Solid lines are the measured isodose curves and dotted lines are the Monte Carlo calculated ones. Different colours represent the isodose levels.
Table 6.3 Shift in the isodose curves in the median-filter denoised DSM calculated data in the diamond-shape field as measured from Figure 6.11.

<table>
<thead>
<tr>
<th>Isodose</th>
<th>mean (mm)</th>
<th>s.d. (mm)</th>
<th>$\Delta_{1.0}$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.95</td>
<td>0.0</td>
<td>0.7</td>
<td>0.7</td>
</tr>
<tr>
<td>0.8</td>
<td>0.9</td>
<td>0.4</td>
<td>1.3</td>
</tr>
<tr>
<td>0.5</td>
<td>0.7</td>
<td>0.4</td>
<td>1.1</td>
</tr>
<tr>
<td>0.2</td>
<td>0.9</td>
<td>0.5</td>
<td>1.4</td>
</tr>
</tbody>
</table>

The median-filter denoised curves are plotted in Figure 6.11 which shows clearly that the isodose curves follow the measurements better than the Gaussian denoised curves. The good agreements are particularly evident in the 0.95 and 0.2 levels. Quantitatively, Table 6.3 shows that the mean shift in the 0.95 curve is 0.0 mm with 0.7 mm standard deviation and the confidence limit ($\Delta_{1.0}$) is 0.7 mm. The mean shift in the 0.2 level curve is 0.9 mm with 0.5 mm standard deviation and the confidence limit ($\Delta_{1.0}$) is 1.4 mm. All confidence limits from the median-filter denoised isodose curves are within the recommended tolerance. In general, these numbers are smaller than those of the raw data and the Gaussian-filter denoised data.

Figure 6.12 is the method noise as seen by the Gaussian (a) and the median filter (b).

Figure 6.12 is the method noise as seen by the Gaussian and the median filter. Structures are clearly visible in both images but the structure in the Gaussian method
noise relates strongly to the MLC leaves (Figure 6.12a) whereas the structure in the median method noise is not as strong as the Gaussian one (Figure 6.12b). The RMS calculated according to Equation 6.4 is $1.2 \times 10^{-2}$ for the Gaussian filter and $1.4 \times 10^{-2}$ for the median filter.

**Discussion**

**MLC penumbrae**

There are two possible causes of the high dose calculated at -15 and 15 cm in Figure 6.7. First of all, the initial electron parameters determined in Chapter 3 may not be suitable for large fields as discussed in Chapter 4 and Chapter 5. Since the field size in this study is $30 \times 36$ cm$^2$ which is larger than the fields tested in previous chapters, it might be possible that there is some over-estimation of the dose. Secondly and perhaps more importantly, the RK chamber is not suitable for measuring small fields (Bucciolini *et al* 2003). In fact it is the large dose gradient that causes the problem. It is likely that the chamber is integrating the dose over a large dimension. The inner radius of the chamber is 2 mm that is oriented along the measuring direction (*cf* Chapter 3 on measurements). Thus the dimension of the chamber (4 mm) is large compared to the 1 cm projected width of one leaf. The measured dose is an average over an area from one penumbra to the next resulting in a gross under-estimation. On the other hand, the calculation comes from voxels of 2 mm in the direction of measurement. The finite volume effect is less severe in the calculated profile.

The second cause is further supported by the data near -12 and 12 cm in Figure 6.7. The open beam area around -12 cm is created by two open leaves while that at 12 cm is created by opening three leaves. The calculation near -12 cm is higher than the measurement but the data match well around 12 cm. For the same reason of averaging over a large dimension, the doses in the leaf umbrae, in both Figure 6.6 and Figure 6.7, are over-estimated by the RK chamber. The calculated penumbrae are likely to be more realistic than the measurements.

On the difference in the magnitudes in the single leaf openings at -15 and 15 cm in Figure 6.7, it is likely to be caused by the asymmetry of the physical leaf profile. The
asymmetry is also evident in the profile near the CAX in both Figure 6.6 and Figure 6.7.

To test the effect of penumbra broadening due to the finite dimensions of the RK chamber, the DSM calculated profiles are convolved with a Gaussian function of zero mean and one standard deviation of the voxel size (2 mm). One standard deviation is chosen because the RK chamber diameter is twice the size of the scoring voxel in the scanning direction; thus the width of the Gaussian function is about the same as the RK chamber diameter. The convolution results are shown in Figure 6.13 and Figure 6.14. Near perfect matches between the RK chamber measurement and the DSM calculation are obtained. The deviations between measurement and calculation are plotted in Figure 6.15.

![MLC profile at 7.5 cm](image)

Figure 6.13 Dose profile across the MLC field at 7.5 cm from the CAX plane. The DSM calculated profile is broadened by a Gaussian function.

If the width of the Gaussian function is measured at half maximum, the width is 2.35 times the standard deviation. Equivalently, the Gaussian function has a width of $2.35 \times 2 \text{ mm} = 4.7 \text{ mm}$ (fwhm).

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8 If the width of the Gaussian function is measured at half maximum, the width is 2.35 times the standard deviation. Equivalently, the Gaussian function has a width of $2.35 \times 2 \text{ mm} = 4.7 \text{ mm}$ (fwhm).
Figure 6.14 Dose profile across the MLC field at -7.5 cm from the CAX plane. The DSM calculated profile is broadened by a Gaussian function.

Figure 6.15 Deviations between the Gaussian-broadened MLC profiles and the RK chamber measurements. The deviations with respect to the dose at CAX (top) are calculated according to Equation 3.1 and the local deviations (bottom) are calculated according to Equation 3.2.
Therefore it is not the initial electron parameters causing the discrepancies between calculation and measurement as shown in Figure 6.6 and Figure 6.7. It is the effect of the large active volume of the RK chamber that causes the problem in the measurement of dose in large gradient regions. In fact, the result here is in line with the analysis by García-Vicente et al (1998) who obtained a Gaussian convolution kernel of zero mean and 2.3 mm standard deviation for the RK chamber measuring the 6 MV beam from an Elekta SL-18 linac.

**Diamond-shaped field**

Studies have shown that the EDR film has very good linearity in dose response up to 350 cGy (Esthappan et al 2002, Chetty and Charland 2002). The dose in this study is 50 cGy and therefore corrections are not required in the conversion from optical density to relative dose. Also, the film agrees with ionisation chamber measurements to 2% in the depth and field size relevant to this study (García-Vicente et al 1998, Chetty and Charland 2002). However, radiographic films tend to over-response in the umbra because of the decrease in primary-to-scatter ratio. Also, radiographic films give sharper penumbra due to its high spatial resolution relative to ionisation chambers (García-Vicente et al 1998). Chetty and Charland (2002) concludes that the overall uncertainty in the radiographic film is in the order of 5%. In a high dose gradient region like the penumbra in this study, 5% uncertainty in dose translates to nearly 1 mm uncertainty in the isodose shift.

The DSM calculated dose distributions, with and without denoising, agree very well with the radiographic films. The shifts in the isodose curves are all within the recommended tolerance of 2 mm. Given that the simulation is carried out with the assumption of water instead of the true elemental composition of the solid water phantom, there is some uncertainty in the dose distribution. Unfortunately, this systematic error is difficult to quantify. Had the true composition been known, the error would largely be eradicated from the beginning. Nevertheless, a simulation with the assumption of polymethyl methacrylate (PMMA) instead of water is carried out to give some idea of the possible systematic error.
Figure 6.16 Isodose curve of the diamond-shape field calculated in PMMA. The calculated curves are shifted inward by 2 to 5 mm compared to the film measurement in solid water. Solid lines are the measured isodose curves and dotted lines are the Monte Carlo calculated ones. Different colours represent the isodose levels.

Figure 6.16 is the plot of the isodose curves from the calculation of the diamond-shape field in PMMA and denoised with the median filter. The calculated curves shift inward by 2 to 5 mm in general. This illustrates that the assumption of water is reasonable in the original simulations. Conversely, the solid water phantom in the experiment is a good approximation to water; it has radiological properties similar to water.

As already shown in the section on MLC penumbra in this chapter, convolving a dose distribution with a Gaussian function amounts to a calculation with a larger scoring voxel. Thus, the volume effect broadens the penumbra. Comparing Figure 6.6 and Figure 6.7 (the raw calculation data) with Figure 6.13 and Figure 6.14 (Gaussian broadened), it is easy to see that much of the statistical fluctuations are removed by the convolution. Denoising with a Gaussian filter is exactly the same operation. The Gaussian filter is an aggressive filter in the sense that the fluctuations are removed
efficiently but at the same time, the dose gradient is also flattened. This effect is equivalent to blurring in image processing.

On the other hand, the median filter is less aggressive in smoothing out the statistical fluctuations but it offers a better preservation of the beam edges. This can be seen in both the confidence limits or the mean shifts as shown schematically in Figure 6.17. Furthermore, the confidence limits from the median filter are generally smaller than those of the Gaussian filter.

![Figure 6.17 Effect on the beam edge by the Gaussian and the median filter as measured by the confidence limits.](image)

Although the median filter shows a slight advantage over the Gaussian one, both types of filters show acceptable performance in terms of the confidence limits in the isodose shifts in this study. In terms of method noise, the median filter is also slightly better than the Gaussian filter. The median method noise resembles more like white noise and structures are less well defined than the Gaussian method noise. On the other hand, the RMS from the Gaussian filter is smaller than that from the median filter. It is because the Gaussian filter performs better in the small dose gradient regions that constitute the bulk of the space. The RMS thus calculated favours the Gaussian filter. In a highly irregular field, it is reasonable to expect that the median filter will out-perform the Gaussian one.

What is not clear is the criteria for choosing the filter parameters. The Gaussian filter in this study has a standard deviation equivalent to 2 scoring voxels while the median
filter computes the median for 5×5 voxels. They are determined by trial and error. Each one represents a compromise between denoising performance and the ability to preserve the beam edges. These decisions are primarily based on visual inspection of the isodose curves. It is difficult to ascertain the amount of systematic error introduced by the denoising techniques to the calculation.

Miao et al (2003) argued that C in Equation 6.2 is actually a function of spatial position and therefore the approach by Deasy (2000) using homomorphic filters which assume that the noise is spatially invariant was insufficient to remove the Monte Carlo noise in a dose distribution; an adaptive filter is necessary. An adaptive filter can detect different regions in an image and modify the filter parameters accordingly.

Chapter summary

In this Chapter, the DSM is applied to two irregular fields shaped by the MLC leaves. In the profile calculations in the MLC field, the DSM results have a better spatial resolution than the RK chamber and therefore the calculated penumbras are narrower and steeper than the measurement. After convolution with a Gaussian kernel (2 mm standard deviation), the calculated profiles match the measurements very well. The Gaussian kernel derived here is also comparable to those found in the literature. It also shows that the DSM is accurate. Regarding the diamond field comparison with the radiographic film, the DSM calculations show average shifts in the isodose curves between 0.8 and 1.0 mm, with confidence limits between 1.3 and 1.5 mm which is within the recommended tolerance. Furthermore, the denoised distributions also exhibit good agreement with the radiographic film. Both the Gaussian and the median denoised distributions have confidence limits less than 1.5 mm in general. The DSM is a good candidate for IMRT calculations.


Chapter 7  Conclusion

Merits of the Monte Carlo method

First of all, the Monte Carlo algorithm is simple. It is the same for different problems provided that they are of the same radiation type. There is no need for a new calculation method for a new problem. There is no theoretical limitation on the complexity of the geometry. Therefore, the Monte Carlo accuracy is only limited by the accuracy of the cross section data and the method of sampling these data. As the research and validation work in these areas progress, the accuracy will only get better over time.

A criticism of using Monte Carlo calculations is that the method does not provide insight into the theories behind the problem. Bielajew (1994) counter-argued that this is just a matter of opinion. Perhaps, the Monte Carlo method should be viewed as a hybrid of theory and experiment. It is a quasi-experimental tool for a theorist and a quasi-theoretical one for an experimentalist. Besides, simulation results may confirm or complement a piece of experimental work. There are situations under which experiments are difficult if not possible; Monte Carlo simulations can predict the results. Landau and Binder (2000) summarise the complementary relationship among simulation, experiment and theory with the following diagram:
Conclusion

It is true that the method requires a lot of computing power. But the advance in hardware and software technology will diminish this limitation. Moore’s Law predicts that computing speed doubles every eighteen months (Moore 1965). An eight-hour simulation today will become a two-hour job in about five years’ time even if there is no improvement in software technique nor any theoretical breakthrough in these five years.

The ultimate error in a Monte Carlo calculation comes from the simplifications in the physics models and cross section data, especially the choice of cross section libraries as discussed in Chapter 2. Therefore, any conclusions based on the microscopic details may not be reliable. They may not represent real nature. On the other hand, the macroscopic results from the simulations can achieve very high accuracy as indicated by many radiotherapy validation studies.

Simulation of the Elekta SLi linac

The Elekta SLi linac has been modelled successfully in this thesis. The geometry has followed the manufacturer’s specification as much as possible. Nevertheless, simplifications, approximations and assumptions are made when necessity arises. For

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9 Moore’s original formulation was to double every twelve months but the figure has been revised subsequently to eighteen months.
example, the MLC leaves are machined to within a certain specified tolerance (about 0.1 mm in most cases). Without actually measuring the physical leaves, it must be assumed that all leaves are exactly the same as each other and the dimensions are as specified in the manufacturer’s drawings. Even this statement ‘as specified in the manufacturer’s drawings’ should be qualified because the model is constructed from a combination of simple planes and quadratic surfaces. The joining of the surfaces are sharp and clear and definite whereas a machined MLC leaf has surfaces joined by some kind of curvatures. Certainly, one does not expect these details to have significant bearing on the simulation results. However, when all the approximations are taken together, the systematic error introduced into the simulations might become significant. Together with the fact that the energy of the bremsstrahlung beam is only a nominal energy, the accuracy of the initial electron beam parameters supplied by the manufacturer is not known with any degree of confidence. Such parameters must be recovered from a series of lengthy trial and error experiments; the dose distributions are simulated under one set of assumed parameters and the results are compared with measurements. Then the simulation is carried out again with some parameters modified and the results re-compared. The process is repeated until the best match is obtained. Therefore, the final set of electron beam parameters includes the deviations of the real, physical linac system from the manufacturer’s specifications, and offsets to counter all the systematic errors introduced to the model by the investigator and the systematic errors in the Monte Carlo codes and cross section data. Strictly speaking, these data are applicable only to the geometry developed in this work, the Monte Carlo codes and the cross section data used in this study. In general, they are comparable to the published results in the literature.

**Phase space models**

As already pointed in various chapters, breaking down the simulations into steps saves computation time, as well as allowing the use of different variance reduction techniques. In particular, it spares the repetition of tracking particles through the patient independent components; it also allows the reuse of particles stored in a phase space file. In MCNP(X), this phase space file is the surface source file. These phase
space files are typically in gigabytes. They are inconvenient to manipulate but their summaries can be very useful. The summary allows the generation of unlimited number of particles. Subsequent simulations are no longer restricted by the number of particles stored in the phase space file. Such a summary is a phase space model. Two well-known models – the point source model (PSM) and the multiple source model (MSM) – have been successfully implemented for MCNP(X) simulations of the patient independent components in this thesis. A third one called the directional spectrum model (DSM) has been developed in this thesis.

Each model has its own advantages and weaknesses. The PSM is easy to implement. It assumes all particles are focused at the electron target. It can be obtained directly during the simulation of the patient independent components. In this case, tallies are placed in the output plane where the phase space is supposed to be. Alternatively, it can be obtained from an existing surface source file that records the particles crossing the output plane. However, its performance is rather poor because it does not account for the scattering of particles by the components.

The MSM is more complex than the PSM. It assumes that particles from a component has a common set of characteristics. Therefore, particle information is summarised for each component. The direction of a particle is determined by the line connecting its position in the component plane to its position on the output plane. Thus the model requires the analysis of the last interaction site of the particle before reaching the output plane. This requirement immediately rules out the generation of the MSM from a simple surface source file that records the particle crossings in the output plane. The MSM is the *de facto* standard in phase space modelling, especially in the simulations with the EGS4 family of codes because the last interaction site information is readily available in the codes and the codes are very popular in linac simulations.

The last interaction site information makes the implementation of the MSM with MCNP(X) particularly difficult. It is because the standard MCNP(X) codes do not keep this piece of information. To find out the last interaction sites, one has to modify the codes or to approximate the last interaction site with the last interaction component. This thesis adopts the latter approach instead of taking the risk of
compromising the integrity of the MCNP(X) codes: the information of the particle’s emergence from each component is recorded in the surface source file and this is done for each particle. Thus the file size grows very fast but little extra information is really included for two reasons. Firstly, many particles emerging from the target and the primary collimator will not reach the output plane at all. They are absorbed by the flattening filter or scattered at a large angle towards a direction of little use. Secondly, of the several surface crossings between the target and the output plane, only one represents the last interaction component. Unfortunately, all crossings must be recorded so that the useful ones can be identified in the post-simulation analysis.

Although the MSM shows superiority over the PSM in principle and in general, the actual results are limited by the MCNP(X) implementation. Nevertheless, the MSM calculated PDD and the dose outside the beam edges agree with the measurements better than the PSM.

The directional spectrum model

The directional spectrum model developed in this thesis overcomes several limitations that the MCNP(X) codes impose on phase space modelling. It does not require the analysis of the last interaction sites. Therefore, a simple surface source file that records the crossings in the output plane is sufficient for the directional spectrum analysis. The immediate consequence is that any phase space with rotational symmetry around the CAX can be used. A phase space that is not originally intended for modelling can be used. Before the development of this model, such phase space can only be modelled with the PSM. Furthermore, all particle data in the phase space are useful. This is in stark contrast to the MCNP(X) generated phase space for the MSM in which only some particle information contributes to the model.

A very interesting property of the DSM is that it directly couples the energy spectrum to the particle direction. In contrast, the MSM has a loose coupling of energy and direction (Verhaegen and Seuntjens 2003) and the PSM does not even
have the directions right. In this sense, the DSM is superior to the other models. The superiority comes at the expense of compactness of the model.

The PSM requires as many energy spectra as the number of radial bins in the output plane. The MSM requires at least three distributions for each component: one spatial distribution in the component plane, one spatial distribution in the output plane and at least one energy spectrum for the component, especially for the flattening filter because off-axis softening of the energy spectrum is evident. For the DSM, there is one energy spectrum for each combination of radial bins and angular deviations from the fan line. However, the end justifies the means here because the DSM calculated dose distributions match the measurements well in the field and outside the field.

**Beam penumbrae**

The beam penumbrae have been investigated with two fields – an irregular field formed by extending several MLC leaves into a large rectangular field (MLC field) and a diamond-shaped field also formed by the MLC leave. In the MLC field, the calculated dose profiles under an MLC leaf is steeper than the measurements with the RK chamber due to the difference in dimensions. The scoring voxels are 2 mm wide in the scanning direction but the RK chamber is 4 mm. With a simple convolution with a Gaussian kernel of 4 mm standard deviation, the calculated profiles agree with the measurements even in the large dose gradient regions. It can be concluded that the DSM performs well even in large fields (the field size set by the diaphragms was 30×36 cm²) and in the presence of the MLC leaves. Furthermore, calculations can be more accurate than the measurement if the wrong choice of chamber is used. The RK chamber is unsuitable for the measurements of penumbrae.

In the diamond-shaped field, the comparison was made with radiographic film. Because the exact elemental composition of the solid water phantom was unknown, ordinary water was assumed in the simulation. The shifts in the isodose curves were measured. The mean shifts and the confidence limits are less than the recommended tolerance of 2 mm. Therefore the DSM calculation is satisfactory. It has the potential of application in the IMRT calculations. Furthermore, digital filters can be very
valuable in the denoising of the Monte Carlo calculated dose distributions. The Gaussian filter is very effective in smoothing the distribution but it tends to smear out the large dose gradient. A median filter preserves the details better.

**Future works**

This thesis is only the beginning of the development of a phase space model that couples the energy to the particle direction. There are many possibilities in the furtherance of the model. First of all, the model has been developed for the 6 MV beam of the Elekta SLi linac. An obvious further investigation is to apply the methodology to different energies and different linac models. Secondly, it is useful as well as interesting to find out whether the DSM can be parameterised. A successful parameterisation will reduce the distributions into a set of values characterising the energy spectra, the angular and the spatial distributions of the particles. It will also point to the possibility of porting the DSM from one linac to another by adjusting the parametric values. This will increase the usefulness of the model because it means that several pre-calculated DSMs will suffice for many linacs. A DSM can be chosen for a new linac based on the dose distributions in the water phantom. It might even be possible to interpolate the parametric values to match the dose distributions for a new linac. Therefore, the simulation of the patient independent components of the new linac can be avoided entirely. The computation time for simulating the patient independent components takes days on a Pentium 4 computer whereas the transport from the output plane to the water phantom takes hours on the same machine. The saving in time is tremendous.

Another line of investigation is in the DSM performance in the prediction of the dose distributions in the small fields, fields smaller than 5×5 cm². It is a necessary step to establish the true usefulness of the model in IMRT. However, the measurements in these small fields are difficult. The use of the RK chamber has been shown by many studies to be inadequate. Pinpoint chambers, diodes and diamond detectors have been investigated by these investigators and found the diamond detectors give the best measurements in the penumbrae. For a true IMRT field, it is also necessary to
investigate the integrated dose over time. In this case, the radiographic films and the portal imagers are indispensable.

Depending on the linac design, there are two IMRT delivery methods, the step-and-shoot method and the dynamic IMRT. As the name suggests, the step-and-shoot method delivers the IMRT field through a series of static fields. On the other hand, the dynamic IMRT delivers the therapeutic beam while the MLC leaves and jaws are in transit. A recent development in the Monte Carlo codes is very exciting in the future IMRT calculations. The Geant4 codes (Agostinelli et al 2003) modified by Paganetti (2004) allow the direct calculation of the dose in proton eye therapy while the beam modulator is in motion. Similar ideas can be extended to the IMRT calculations. A new feature called stochastic geometry in MCNP5 (Brown et al 2005) should also be investigated for such purposes.

The application of MCNP(X) seems to be gaining momentum in the medical physics community in recent years. It is easy to use, powerful and well validated. However, the Geant4 codes with the recently available low energy module (Carrier et al 2004) should not be ignored. It is in many ways as powerful as the MCNP(X) codes. It also supports tracking of electrons in electromagnetic fields. This option will open up many possible investigations in the linac simulations (Raaymakers et al 2004). Of course, the DSM performance with the new codes under different simulation conditions requires further assessments and validations.

In any Monte Carlo calculation, statistical fluctuations are unavoidable. Denoising techniques should be studied further because it has the potential to be a powerful variance reduction technique as argued by Kawrakow (2002). The image processing community has developed a large number of digital filters. Apparently, many of these filters can be directly imported into the denoising of the Monte Carlo calculated dose distributions. The application of the non-local means filter in motion pictures has been shown to be promising (Buades et al 2005b). Its application to denoising 3D Monte Carlo dose distributions seems to be a reasonable extension. It might even be possible to denoise 4D distributions. The non-local means filter warrants further studies.
Further studies should also be carried out to establish the noise model. At the time of writing of this thesis, the best model available is the Gaussian model suggested by Sempau and Bielajew (2000). In the derivation of the model, the authors clearly point out that it is a good approximation with the electron transport turned on. Although an accurate calculation should include the electron transport, it is of great interest and usefulness if the computationally expensive electron transport can be turned off. In this case, a noise model is yet to be established. It should be exciting as well because a successful model ought to take into account of the systematic errors arisen out of the omission of the electron transport.

This last point brings the discussion on dose calculations back to a full circle – we want to use the Monte Carlo method in treatment planning calculations because it is accurate. It is accurate because it models all the necessary physics. The electron transport has a very important role to play in it. Photon energy is deposited through the electrons. The superposition/convolution method fails near heterogeneities and tissue boundaries precisely because these locations are where the electronic disequilibrium occurs. Can a noise model overcome the lack of electronic equilibrium?
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Appenda

Publications

Alghamdi AA, Ma A, Marouli M, Albarakati Y, Kacperek A and Spyrou NM 2006
High resolution anthropomorphic voxel-based tomographic phantom for proton therapy
of the eye. *Physics in Medicine and Biology* (submitted)

Ma A, Awotwi-Pratt J, Alghamdi A, Alfuraih A and Spyrou NM 2006 Monte Carlo
study of photoneutron production in the Varian Clinac 2100C linac. *International Journal
of Radioanalytical and Nuclear Chemistry* (submitted)

Alghamdi A, Ma A and Spyrou NM 2006 Calculation of photonuclear yield using an
anthropomorphic phantom by Monte Carlo simulation. *International Journal of
Radioanalytical and Nuclear Chemistry* (accepted for publication)

Alfuraih A, Alghamdi A, Ma A and Spyrou NM 2005 Prospect of using the photoneutron
beam component from high energy linacs in BNCT, a Monte Carlo simulation.
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Alghamdi A, Ma A, Tzortis M and Spyrou NM 2005 Neutron fluence-to-dose conversion
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Ma A, Awotwi-Pratt J, Alghamdi A, Alfuraih A and Spyrou NM 2006 Monte Carlo
study of photoneutron production in the Varian Clinac 2100C linac. 7th International
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Conference on Methods and Applications of Radioanalytical Chemistry, Kona, Hawaii, USA, 3rd–7th April 2006 (poster)

Alfuraih A, Ma A, Alghamdi A and Spyrou NM 2006 Prospects of high energy medical linear accelerators in BNCT, a Monte Carlo simulation using voxelised phantom. 7th International Conference on Methods and Applications of Radioanalytical Chemistry, Kona, Hawaii, USA, 3rd–7th April 2006 (poster)


Alghamdi A*, Ma A, Marouli M, Alkhraif M, Prekas G, Alfuraih A and Spyrou NM 2005 Simulation of high resolution eye phantom for proton therapy. The 8th International Conference on Nuclear Analytical Methods in the Life Sciences, Rio de Janeiro, Brazil, 17th–22nd April, 2005 (oral)

Alfuraih A*, Ma A and Spyrou NM 2005 Boron neutron capture therapy using medical linear accelerator. The 8th International Conference on Nuclear Analytical Methods in the Life Sciences, Rio de Janeiro, Brazil, 17th–22nd April, 2005 (oral)


Ma A and Spyrou NM 2004 A directional spectra approach to phase space modelling of a 6 MV beam from a medical linear accelerator. Advanced Workshop on Current Topics in Monte Carlo Treatment Planning, McGill University, Montreal, Canada, 3rd–5th May 2004 (poster)
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**Co-supervised MSc Medical Physics dissertations**

Chan KH GEANT4 application in the characterisation of the metal plate/phosphor screen of an a-Si:H electronic portal imaging device. University of Surrey, 2005, co-supervised with Dr DG Darambara

Myronakis M Monte Carlo simulations of a small animal SPECT system using GATE. University of Surrey, 2005, co-supervised with Dr DG Darambara

Dubicki J A directional spectrum model of a 6 MV photon beam from a medical linear accelerator. University of Surrey, 2004, co-supervised with Prof NM Spyrou

Tzortzis M Neutron dosimetry calculations using an anthropomorphic realistic model and the MCNP4C Monte Carlo code. University of Surrey, 2003, co-supervised with Mr A Alghamdi and Prof NM Spyrou