Efficient Monte Carlo simulations
in kilovoltage x-ray beams

by

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Abstract

Kilovoltage x-ray systems are modeled with BEAMnrc using directional bremsstrahlung splitting, which is five to six orders of magnitude more efficient than a simulation without splitting and 60 times more efficient than uniform bremsstrahlung splitting. Optimum splitting numbers are between 2 and 3 orders of magnitude larger than for megavoltage beams.

A self-consistent approach for the calculation of free-air chamber correction factors with the EGSnrc Monte Carlo system is introduced. In addition to the traditional factors employed to correct for attenuation (A_{att}), photon scatter (A_{scat}) and electron energy loss (A_{eloss}), correction factors for aperture leakage (A_{ap}) and backscatter (A_{b}) are defined. Excellent agreement is obtained between calculated and measured A_{scat} and A_{eloss} values. Computed A_{att} values for medium-energy and mammography beams reproduce the measurements well. For low-energy lightly-filtered beams, A_{att} values show significant differences with the experiment. Scaling the tungsten L-shell EII cross-sections by a factor of 2 eliminate these differences. The inconsistency of the evacuated-tube technique for measuring A_{att} is negligible for medium-energy and mammography beams, and 0.2% for low-energy lightly-filtered beams. The aperture correction A_{ap} becomes significant in the medium-energy range with increasing energy. The newly introduced backscatter correction A_{b} becomes as high as 0.4% in the low-energy range.

In the medium-energy range, calculations reproduce experimental half-value layer values to better than 2.3%. For mammography beams a difference of 0.5% and 2.5% with experiment is obtained with and without a scaling of the tungsten L-shell EII cross-sections respectively. For low-energy lightly-filtered beams a scaling factor of 2.1 gives the best agreement ($\sim 3\%$) with the experiment, significantly worsening

to 8% for a scaling factor of 1.8, which gives the best match for A_{att} .

The fast algorithm for calculating the scatter contribution to cone beam computed tomography scans increases the efficiency by more than 3 orders of magnitude. Smoothing the scatter distribution pushes the efficiency gain over four orders of magnitude. The iterative correction algorithm removes the scatter from the measured scans improving the accuracy of the reconstructed image. The dependence of image reconstruction accuracy on the sophistication of the photon interaction models is investigated. No significant difference is observed when using models including coherent and incoherent scattering. Considering only incoherent scattering for free electrons shows a significant bias.

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Back in 1992, Dr. Roberto Capote dropped an EGS4 manual on my lap and asked me if I was interested in doing some Monte Carlo simulations for him. I hold him responsible for my involvement with EGS. A huge debt of gratitude goes to him for his guidance and support in moments of great uncertainty.

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Statement of Originality

This thesis describes the author's research during the course of the Ph.D. program at Carleton University. This work was conducted at the National Research Council of Canada. Many of the results herein have been presented at local seminars organized by the Ottawa Medical Physics Institute (OMPI) and international conferences. The main results of this thesis have been summarized in a set of papers published in the journal Medical Physics, the official journal of both the Canadian Organization of Medical Physicists (COMP) and of the American Association of Physicists in Medicine (AAPM) and in the journal Physics in Medicine and Biology, the official journal of many international medical physics societies such as the Deutsche Gesellschaft für Medizinische Physik, the Japanese Association of Radiological Physics, the European Federation of Organisations for Medical Physics, the International Organization for Medical Physics, and COMP as well. The following list details the papers in chronological order describing where the results are found within this thesis, as well as the author's contributions to each paper:

- E. Mainegra-Hing and I. Kawrakow. Efficient x-ray tube simulations. Medical Physics (33), 2006, 2683-2690.
 - The contents of this paper constitute Chapter 3 where the efficiency of directional bremsstrahlung splitting for x-ray beams is discussed and a methodology for finding optimum DBS parameters is presented.
 - The author performed all of the calculations for this paper and drafted and performed edits on the manuscript.

- E. Mainegra-Hing and I. Kawrakow. TU-D-224C-08: Effect of Different Physical Processes and Data Sets On HVL Calculations. Medical Physics (33), 2006, 2200.
 - The results of this study appear in section 5.2 of Chapter 5 discussing the need to use the most accurate photon interaction model with the best cross-section data compilation for accurate HVL calculations.
 - The author performed all of the calculations and presented the results as an oral presentation at the 48th AAPM annual meeting in 2006.

- E. Mainegra-Hing and N. Reynaert and I. Kawrakow. Novel approach for the Monte Carlo calculation of free-air chamber correction factors. *Medical Physics* (35), 2008, 3650-3660.
 - The methods and results of this paper appear in Chapter 4 where a self-consistent set of FAC correction factors is derived, its implementation in the user code `egs_fac` described, and the results for medium-energy beams presented.
 - The author performed most of the calculations for this paper with the exception of the calculations for A_{cpe} and A_x and drafted and performed edits on the manuscript.

- E. Mainegra-Hing and I. Kawrakow. Fast Monte Carlo calculation of scatter corrections for CBCT images. *Journal of Physics: Conference Series* (102), 2008, 012017.
 - The methods and results of this paper appear mostly in section 6.4 of Chapter 6 describing the scatter correction algorithm and its ability to faithfully reproduce test phantoms.
 - The author performed all of the calculations for this paper, drafted and performed edits on the manuscript, and presented the results as an oral presentation at the III McGill International Workshop on Monte Carlo Techniques in Radiotherapy Delivery and Verification in 2007.

- E. Mainegra-Hing and I. Kawrakow. TU-EE-A4-05: Influence of Photon Scatter Modeling On Image Reconstruction Accuracy in CBCT. *Medical Physics* (35), 2008, 2914.
 - The results of this study appear in section 6.7 of Chapter 6.
 - The author performed all of the calculations and presented the results as a moderated poster at the 50th AAPM annual meeting in 2008.

- E. Mainegra-Hing and I. Kawrakow. Variance reduction techniques for fast Monte Carlo CBCT scatter correction calculations. *Physics in Medicine and Biology* (55), 2010, 4495-4507.
 - The variance reduction techniques used in this paper are presented in section 6.2 and the results in section 6.6.2 of Chapter 6.
 - The author performed all of the calculations for this paper and drafted and performed edits on the manuscript. These results were presented at the Second European Workshop on Monte Carlo Treatment Planning in 2009 in an oral presentation prepared by the author and given by Dr. Iwan Kawrakow. (Travel restrictions prevented the author from attending the meeting).

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List of Acronyms

AEIT	Approximated Efficiency Improving Technique
BCSE	Bremsstrahlung Cross Section Enhancement
DBS	Directional Bremsstrahlung Splitting
EII	Electron Impact Ionization
FAC	free-air chamber
FS	Fixed Splitting
HVL	Half-Value Layer
IAA	Independent Atom Approximation
IAAFF	Independent Atom Approximation Form Factors
IGRT	Image Guided Radiation Therapy
IMRT	Intensity Modulated Radiation Therapy
LASG	locally-adaptive Savitzky-Goley
MAPE	Mean Absolute Percentage Error
MC	Monte Carlo
MCSFF	Molecular coherent scattering form factors
MRE	Mean Relative Error
MFPTR	Mean Free Path Transform

\$MXGE	maximum number of photon energy points
PDIS	Position Dependent Importance Splitting
POM	point of measurement
RIA	Relativistic Impulse Approximation
RMSE	Relative Root Mean Square Error
RR	Russian Roulette
rr	range rejection
RT	Radiation Therapy
SBS	Selective Bremsstrahlung Splitting
UBS	Uniform Bremsstrahlung Splitting
VRT	Variance Reduction Technique
xVMC	Photon Voxel Monte Carlo

Chapter 1

Introduction

1.1 General introduction

After more than 100 years of x-ray use in medicine, science and industry, it is undeniable the great impact x-rays have had for mankind. Today, x-rays find a wide range of applications in areas such as medicine, non-destructive sample analysis, crystallography, airport security, food inspection, and lithography, to only name a few. Immediately after their discovery, x-rays found medical application not only in diagnostic radiation imaging, but also in radiation therapy (RT). External RT technology was dominated in the first half of the 20th century by kilovoltage x-ray machines. The drive for higher energies and intensities lead to the development of Co-60 machines in the late 1950s and soon thereafter to the introduction of linear accelerators (linacs). Nowadays, kilovoltage x-ray beams are mostly used in medicine for diagnostic imaging, mammography, and some superficial skin irradiations.

Imaging x-ray systems are being increasingly used in RT with the advent of sophisticated RT techniques. The introduction of 3D conformal RT techniques¹⁻³

such as intensity-modulated RT⁴⁻⁹ (IMRT) has driven the development and introduction of x-ray imaging tools and techniques in RT. Radiation imaging and RT are becoming tightly inseparable as the need for accurate patient anatomical and positional information becomes critical for adaptation to the dynamic nature of the RT processes. Image-guided RT¹⁰⁻¹⁴ (IGRT) uses patient imaging in the treatment room to increase the conformality of the radiation dose to the tumor, improving tumor control and reducing normal tissue complications. To account for changes in tumor size due to treatment and for patient anatomical variations, such as rigid body motion, organ filling and patient respiration during the RT process, IGRT is moving rapidly towards adaptive RT¹⁵⁻¹⁷ (ART). Using different imaging modalities, varying anatomical patient parameters, as well as the treatment dose can be estimated and fed back to the treatment planning system (TPS) for adaptive re-planning. Miniature x-ray tubes are finding application as substitute to radionuclide-based brachytherapy seeds in the emerging new field known as electronic brachytherapy (eBx).¹⁸⁻²⁰ These eBX sources apply interstitial irradiation which can be user-adjusted (on/off) without the radioactive waste concerns connected with radionuclides. With the improvement of electronic portal imaging devices (EPID) and the introduction of flat-panel detector (FPD) technologies in the 1990s, the number of x-ray machines in use at the clinic rose significantly.²¹ Hence, it is not surprising that with all these novel developments and a renewed interest in RT with superficial and ortho-voltage x-rays, x-ray machines have become an important component of the RT setup.

A proper characterization of the x-ray beam is crucial for the development and efficient use of x-ray systems. The most accurate way of specifying a kilovoltage x-ray beam is through knowledge of the photon spectrum. Experimental measurement of an x-ray spectrum requires special equipment, only available in a limited number of laboratories. Since these measurements are time consuming and very difficult, different calculational approaches for estimating x-ray spectra have been developed.

1.1. GENERAL INTRODUCTION

The photon spectrum produced by an x-ray tube depends on the tube potential, target angle, material and thickness of the target, window and filter, among other factors. Empirical and semi-empirical models are adjusted to reproduce a limited set of beam qualities (preset target/filter combinations) and thus cannot be relied on when studying newly developed x-ray systems. Although these models still remain the fastest methods for x-ray spectra estimation, the models proposed so far still have limitations. In the Monte Carlo (MC) simulation of an experimental setup, all available information can be included to create a realistic model. All possible photon interactions (coherent scatter, incoherent scatter and photoelectric absorption) in the kilovoltage energy range are considered in the simulation, accounting for attenuation and scatter in the different components of the experimental setup. For these reasons, MC modeling remains the only alternative to overcome the limitations of empirical and semi-empirical models, making it an excellent tool for the accurate characterization of x-ray systems.

1.2 Motivation

The main drawback of an x-ray beam MC simulation is the long times associated with simulating the emission of bremsstrahlung photons in the kilovoltage energy range. Since this process is very rare at these energies, a large number of MC particle histories are necessary to generate enough bremsstrahlung to achieve a reasonably small statistical uncertainty. In this work, we describe the development and implementation of techniques for improving the efficiency of the simulation of x-ray systems using the MC simulation system EGSnrc.²² The meaning of efficiency is made clear in section 2.1.1. From the x-ray generation in the target and transport through the collimation system, we move on to simulating their transport through measuring devices such as

free-air ionization chambers (FAC) and realistic phantoms.

We start with the basic simulation of an x-ray tube system and find the optimum parameters for the efficient modeling of narrow x-ray beams using a Variance Reduction Technique (VRT) known as Directional Bremsstrahlung Splitting (DBS).²³ For a brief introduction to VRTs, the reader is referred to section 2.2. Once we can simulate an x-ray beam efficiently, we proceed to benchmark our x-ray tube model against the experimental determination of the Half-Value Layer (HVL). Task Group 61²⁴ (TG-61) of the American Association of Physicists in Medicine (AAPM) recommended the HVL as the beam quality specifier to be used in combination with the tube potential, providing compilations of dosimetric data as a function of this quantity. The availability of high quality experimental HVL data at our lab offers a great opportunity to validate the accuracy of the simulations. Potential sources of discrepancies with the experiment will come from the ability to produce accurate x-ray spectra and from uncertainties in the total photon cross sections.

But before calculating HVL values, one needs to determine a set of correction factors for the parallel-plate FACs used for the HVL measurement and air-kerma based calibration of ionization chambers. Since accurate determination of the air-kerma is required in both cases, this set of correction factors is needed to convert the detector signal into air-kerma. Most of the individual corrections have a 0.5 % effect or less, hence one needs to implement methods for the efficient calculation of these corrections to a small enough statistical uncertainty (less than 0.01 %). In this work, a self-consistent set of FAC corrections factors is theoretically derived. An algorithm for their calculation using the MC method is described which makes use of sophisticated VRTs that significantly increase the efficiency of the calculations.

HVL can be extracted from FAC measured attenuation curves. The largest correction needed is the attenuation correction A_{att} , which can be about 1% at medium

1.2. MOTIVATION

energies and as large as 3% in the low-energy range. The relative variation of the air-kerma with attenuator thickness is measured at distances larger than 50 cm from the x-ray source in a scatter free, “narrow beam” setup. In the experimental setup used for the HVL determination at our lab, the point of measurement (POM) is defined at 1 m from the x-ray source.

The more stringent accuracy requirements in current novel RT techniques for computing dose distributions in TPSs and estimating corrections for dose measuring and imaging devices can only be met with the use of MC techniques. However, the clinical community has disregarded the use of MC-based algorithms given the long calculation times usually needed. The ever increasing computing power (faster and cheaper computers) and the development of very efficient MC algorithms have led to a progressive inclusion of MC techniques in the clinical environment. TPSs are starting to incorporate fast MC algorithms to accurately compute the dose for complex treatment setups where conventional algorithms fail to produce accurate enough results.²⁵ Kilovoltage cone beam computed tomography (CBCT) is used as an imaging guiding tool for IGRT.²⁶ There is still an active debate whether kilovoltage or megavoltage CBCT is better suited for IGRT.²⁷ Although kilovoltage CBCT provides much better quality images and a smaller imaging dose, megavoltage CBCT is simpler to implement since it uses the x-rays directly from the linear accelerator (LINAC) used to treat the patients. Due to the much higher scatter for kilovoltage CBCT compared to megavoltage CBCT, the advantage of using kilovoltage CBCT remains questionable unless an efficient and accurate way of correcting kilovoltage CBCT images is implemented. MC simulation can be used to faithfully model the patient setup and produce an accurate estimation of the scatter distribution. In this work, a MC-based algorithm for the fast estimation of the photon scatter contribution from the patient geometry to CBCT scans is described and applied to different phantoms.

1.2. MOTIVATION

1.3 Outline of the thesis

Chapter 2 introduces the MC method in radiation transport and describes EGSnrc, the MC simulation system used for the calculations. Extensions to EGSnrc are described which allow for more flexible use of user-supplied data such as photon cross sections, Electron Impact Ionization (EII) cross sections and coherent scatter form factors. An extension to the EGSnrc user-code BEAMnrc^{28,29} is described which allows the estimation of air-kerma at a scoring plane for an user-defined field.

Chapter 3 describes a procedure to optimize the simulation of x-ray tube systems for narrow beam geometries using DBS. This VRT was implemented in BEAMnrc, an EGSnrc user-code widely used for the simulation of megavoltage medical linacs. BEAMnrc provides an optimized geometry implementation that can be used to model x-ray tubes and was therefore selected for this work.

In Chapter 4, a self-consistent set of parallel-plate FAC correction factors for x-ray beams is theoretically derived. Correction factors for the Low Energy Exposure Standard (LEES) and Medium Energy Exposure Standard (MEES) FACs in use at the Ionizing Radiation Standards (IRS) group of the National Research Council of Canada (NRC) are calculated and compared to available experimental values.

In Chapter 5, the IRS setup for attenuation measurements with a FAC is modeled accurately in order to reproduce HVL measurements. HVL is the quantity recommended in TG-61²⁴ as the x-ray beam quality specifier. Poor agreement between MC calculated and measured values have been reported in the literature.³⁰⁻³² The FAC correction factors from the previous chapter are used to correct the calculated FAC reading in a similar fashion as done in experimental HVL determinations. The agreement between experimental and MC calculated HVL values obtained provides a validation of the techniques and algorithms used.

In Chapter 6 a very fast MC algorithm for scatter correction in CBCT imaging is described and benchmarked. Especial attention is given to the different `splitting + Russian roulette` algorithms developed since these produce the largest efficiency gains from all VRTs used.

General conclusions are presented in Chapter 7 with a discussion of future work that will be carried out based on the results presented here. Most of the techniques and algorithms developed in this work are available through the EGSnrc user-codes cavity, `egs_fac` and `egs_cbct` which are freely available, except `egs_cbct`, which has not been released yet.

Chapter 2

Methods and materials

2.1 Monte Carlo simulation of radiation transport

Simulation is defined as a technique of performing sampling experiments on the model of a system.³³ This is often called simulation in a wide sense, whereas simulation in a narrow sense, or stochastic simulation is actually a statistical sampling experiment with the model. Because sampling from a probability distribution involves the use of random numbers, stochastic simulation is also known as Monte Carlo simulation. The term “Monte Carlo” simulation dates back to 1944 when von Neumann and Ulam used it as a code word for their secret work on the atomic bomb at Los Alamos during World War II. It was suggested by the gambling casinos from the city of Monte Carlo in Monaco.

Historically, the MC method was used successfully for the first time to solve particle transport problems using electronic computing techniques and this still is one of the areas of most extensive use.³⁴ There is a vast literature available on the subject of MC simulation. For a general introduction to the method, the user is referred

to the excellent monographs on MC by Sobol,³⁵ Hammersley and Handscomb³⁶ and Rubinstein.³⁷ Basic references for the application of the MC method to the simulation of radiation transport are for instance the books by Lux and Koblinger,³⁴ Cashwell and Everett³⁸ and a compendium of lectures on MC transport of electrons and photons taught in Erice, Italy and published as a reference book, known as the “orange bible”, by Jenkins *et al.*³⁹ The review chapter by Andreo⁴⁰ is also a very useful source on this topic.

Simulating the transport of photons and electrons requires modeling a source, a transport geometry and all relevant interaction processes. The initial particle type, energy and direction are sampled from the probability distributions associated with the source. Once the initial conditions for a given MC history are set, the distance d to the next interaction is sampled from the corresponding probability distribution. The particle is then transported a distance d (with or without losing energy) taking the particle to a collision site or outside the geometry, terminating the history. At the collision site the interaction type is selected based on interaction cross sections for this particle. The particle can be absorbed or scattered (changing its energy and/or direction), possibly creating additional particles. This “shower” of secondary particles is completely simulated in a similar fashion until all particles “die” as a result of a catastrophic interaction, lose enough energy so they cannot escape a certain region or leave the geometry. Quantities of interest are obtained by averaging over a large number of particle histories thus obtaining an estimate of this quantity with an associated statistical uncertainty.

The first comprehensive discussion of a photon transport simulation was given by Kahn.⁴¹ In general, the simulation of photon transport is much easier than the simulation of charged particles because the simulation can be done in an analog way (i.e., every interaction is explicitly simulated) and the cross sections are well

2.1. MONTE CARLO SIMULATION OF RADIATION TRANSPORT

known when electron binding effects can be neglected or treated with relatively simple models, a situation encountered in a wide range of applications.

The simulation of electron transport however requires a different approach. While photons interact only a relatively few times and follow straight paths, electrons suffer of the order of millions of elastic and inelastic interactions when slowing down from typical RT energies (megavoltage energy range) following very tortuous paths. Modeling all these interactions and keeping track of all secondary particles generated in an analog fashion would be impractical even with current available computing power. In 1963, Berger⁴² introduced the condensed history technique (CHT) that allowed the efficient simulation of electron transport by grouping electron interactions into single “steps” that account for the cumulative effect of elastic and inelastic collisions. To this end, one needs to sample energy, direction, and position changes from appropriate distributions of grouped single interactions, e.g., multiple scattering, stopping power, etc. This technique is based on the fact that most of the electron interactions lead to very small changes in the electron energy and/or direction. CHT is the basis of all modern electron-photon transport MC codes relevant to medical physics.

2.1.1 Efficiency of a MC simulation

The statistical uncertainty associated with a MC simulation can be made as small as desired by increasing the sample size N . However, this straightforward approach is not very practical as the statistical uncertainty σ is inversely proportional to the square root of the sample size N according to the central limit theorem.^{43–45} Thus, to reduce the statistical uncertainty by a factor of 10, one would have to run 100 times more MC histories. For this reason, a MC algorithm should be designed in such a manner that it extracts as much information as possible, with the least possible

amount of effort. With such a well designed MC algorithm, one can estimate the quantity of interest with a desired statistical uncertainty in an efficient way.

Throughout this work, efficiency will be taken as inversely proportional to the product of the sample standard deviation squared s^2 and the calculation time T required to obtain this estimate, i.e.,

$$\varepsilon = \frac{C}{s^2 \cdot T}, \quad (2.1)$$

with C an arbitrary constant, which in this work has been taken to be the sample mean squared. Hence efficiency is obtained from the relative error and given in units of inverse time.

Since s^2 is inversely proportional and T is directly proportional to the sample size N , the MC efficiency ε is independent of N for a given MC model. This way of defining efficiency provides a measure of how fast a quantity can be estimated to a desired statistical uncertainty under the same material conditions. An efficient MC simulation produces an estimate of the quantity of interest either by sacrificing calculation time to achieve a drastic reduction in the sample variance or reducing calculation time without significantly increasing the variance. Variance Reduction Techniques (VRTs) increase the efficiency by modifying the underlying probability distributions without introducing a bias into the estimation, thus making the results more precise without sacrificing reliability.

2.2 Used Variance Reduction Techniques (VRTs)

The continuous development of VRTs allows the solution of problems which had been deemed impractical to tackle due to excessively large computation times. According

to Eq. (2.1), an efficiently implemented VRT reduces the computing time needed to achieve a desired statistical uncertainty. Although one might think that with increasing computer power there is no need to develop new or improve existing VRTs, this increased computing power allows tackling new, more challenging, problems which again brings this very computing power to its limits. Moreover, the inclusion of more detail for realistic simulations and the drive for even smaller uncertainties makes the use of VRTs still a necessity. With the development of very sophisticated VRTs one can increase the calculation efficiency by several orders of magnitude which, with only sheer computing power, would be costly or in some cases impossible to achieve.

A large number of VRTs to improve the efficiency of MC simulation of radiation transport have been developed. This long list includes techniques such as interaction forcing, exponential path length biasing, Russian roulette, correlated sampling, particle splitting, just to mention a few. The references in section 2.1 describe many of these techniques in detail. The reader is also referred to the publications by Bielajew and Rogers,^{46,47} Kawrakow and Fippel,⁴⁸ and Sheikh-Bagheri *et al.*⁴⁹ The following subsections provide a brief description of VRTs used in this work. Some of them are variations or combinations of well known VRTs such as path length biasing, particle splitting and Russian Roulette (RR).

2.2.1 Photon interaction splitting

The combination of particle splitting with RR has proven to be a powerful tool for increasing the efficiency of external photon beam simulations in RTP by up to a factor of 5.⁴⁹ Fast MC simulation systems such as VMC/xVMC^{48,50} and VMC++⁵¹⁻⁵⁴ have incorporated photon interaction splitting with RR to achieve a more uniform distribution of photon interaction sites and reduce the time spent following secondary photons. Each photon is split into N_{split} photons which interact at different loca-

2.2. USED VARIANCE REDUCTION TECHNIQUES (VRTS)

tions spread along the photon's direction. The number of mean-free-paths for the i^{th} photon, η_i , is calculated from

$$\eta_i = -\ln \left(1 - \frac{\xi + i - 1}{N_{\text{split}}} \right), \quad (2.2)$$

where i runs from 1 to N_{split} and ξ is a random number, uniformly distributed between 0 and 1. Each photon carries a fraction of $1/N_{\text{split}}$ of the statistical weight w_0 of the initial photon. Since $\eta_i > \eta_{i-1}$, only transport from η_{i-1} to η_i is necessary to get to the interaction site of the i^{th} interaction. This approach enables the transport of N_{split} photons with a single pass through the geometry.

This technique has been dubbed SPL and is more efficient than photon interaction forcing alone or combined with splitting.⁴⁸ SPL is also used in the EGSnrc voxel-based dose calculation user-code DOSXYZnrc.⁵⁵ A more modest increase in efficiency of up to a factor of 3 has also been obtained with SPL in the calculation of ionization chamber response. This efficiency increase is still significant and hence SPL has been implemented in the EGSnrc user-codes for ionization chamber simulation CAVRZnrc,⁵⁶ `cavity`, `egs_fac` and `egs_chamber`.⁵⁷

2.2.2 Directional Bremsstrahlung Splitting (DBS)

Directional Bremsstrahlung Splitting²³ (DBS) was implemented in the BEAMnrc code⁵⁸ to further improve the efficiency of photon accelerator simulations over previous bremsstrahlung splitting techniques such as Uniform Bremsstrahlung Splitting²⁸ (UBS) and Selective Bremsstrahlung Splitting^{59,60} (SBS). With DBS, bremsstrahlung photons aimed at a user-defined surface, where the quantity of interest is scored (scoring field), are normally transported. Photons, whose direction does not intercept with the scoring field are subjected to a RR game. The survival probability of this

2.2. USED VARIANCE REDUCTION TECHNIQUES (VRTS)

RR game is chosen in such a way that, on average, only one photon survives. This scheme reduces the number of transported photons not contributing to the scoring and guarantees that all photons reaching the scoring field will have the same weight. Although its name suggests that only bremsstrahlung events are split, DBS uses a combination of interaction splitting with RR for secondary electrons and photons not only for bremsstrahlung, but also for annihilation, Compton scattering, pair production and photo-absorption. Moreover, *a priori* knowledge of the probability for photons to reach the scoring field after these interactions is used to reduce the number of interactions sampled.

DBS was shown to be over 20 times more efficient than UBS for calculating the photon fluence of a 6 MV photon beam from an Elekta SL25 accelerator and a 10×10 cm² field at 100 cm from the bremsstrahlung target. The efficiency gain observed in the megavoltage energy range using DBS suggests that this technique can significantly increase the calculation efficiency for kilovoltage beams over UBS, the VRT employed by most previous EGS4/BEAM investigations.

2.2.3 Photon interaction splitting and RR for scatter calculations

Similarly as in subsections 2.2.1 and 2.2.2, a combination of interaction splitting with RR can be used to improve the efficiency in the estimation of the scatter contribution from an x-ray beam. The main difference with the method in 2.2.1 is that here, the interaction is sampled N_{split} times at the same interaction site. Unlike DBS, this technique is used for a photon-only simulation. All N_{split} interactions are simulated, although N_{split} does not have to be constant. N_{split} can be selected before each photon interaction proportional to the potential contribution of the photon to the signal or

2.2. USED VARIANCE REDUCTION TECHNIQUES (VRTS)

based on the the importance region the photon is currently in. This VRT is used in Chapter 6 for estimating the scatter contribution to CBCT scans. Several schemes for selecting the splitting number N_{split} are developed in that chapter and their effect on the efficiency is studied. Scattered photons aimed at the scoring field are kept and followed normally, while those not aimed at the scoring field are subjected to a RR game.

2.2.4 Range rejection with RR

Range rejection (rr) is not a true VRT since it introduces an approximation by neglecting residual bremsstrahlung or annihilation photons. For this reason, it belongs to a different category of algorithms known as Approximated Efficiency Improving Techniques (AEITs). When a charged particle cannot reach a region of interest due to energy considerations based on its residual range, its history is terminated and the particle is considered to deposit its energy on the spot. This technique can save significant computing time when the contribution from the bremsstrahlung and annihilation photons is negligible.

Alternatively, one can combine rr with Russian Roulette (RR), whereby charged particles are not discarded, but subjected to a RR game with a probability p . Surviving particles will carry a statistical weight increased by a factor of $1/p$. Any photon generated by these surviving charged particles will represent all photons that would have reached the region of interest by having an increased statistical weight. Since this technique is combined with the splitting technique from section 2.2.1, any of these heavy weight photons will be subjected to splitting into $1/p$ photons. This technique is a true VRT and has been used here in all the simulations concerning the modeling of ionization chambers. Kawrakow⁶¹ reported a factor of 5 efficiency increase in the megavoltage energy range when computing the dose to the cavity of an ionization

2.2. USED VARIANCE REDUCTION TECHNIQUES (VRTS)

chamber placed in a water phantom.

2.2.5 Correlated sampling (CS)

Correlated sampling is a useful technique when the quantity of interest can be calculated as the ratio or difference of two strongly correlated quantities. This is the case for instance when computing correction factors for ionization chambers. These correction factors are usually calculated as the ratio of the dose to the chamber cavity for two slightly different geometries (different wall material or thickness, electrode material, etc.). By designing the MC calculation in such a way, that both quantities can be computed at the same time, one can make use of the same sequence of random numbers and similar particle trajectories, which guarantees a very strong positive correlation. Since the variance of the ratio of two correlated quantities equals the sum of their variances minus a term directly proportional to the covariance between them, it will have a much smaller uncertainty than if one computed these quantities independently. The use of correlated sampling for radiation dosimetry applications is extensively described elsewhere by Holmes *et al.*,⁶² Ma and Nahum^{63,64,64–66} and Buckley *et al.*⁶⁷

2.2.6 Forced detection (FD)

Often one needs to estimate the photon fluence $\psi(E)$ or a fluence-dependent quantity such as the kerma K at a defined scoring region (planar or volumetric). The usual approach is to compute the individual contribution from photons crossing the scoring region. This is already more efficient than the kerma approximation where a full simulation of all photon interactions is performed assuming electrons deposit their energy on the spot.

2.2. USED VARIANCE REDUCTION TECHNIQUES (VRTS)

One can go one step further and estimate the contribution to the kerma from any photon that could potentially cross the scoring region. An algorithm to determine whether the direction of the photon intercepts with the scoring region needs to be implemented, as well as an exact ray-tracing algorithm to account for the attenuation through the geometry. This way, one does not have to wait until the photon reaches the scoring region to estimate its contribution to the kerma and a more efficient sampling of all possible contributions is achieved. This approach is equivalent to running N separate MC simulations where in the i^{th} simulation, only the contribution to the kerma from particles interacting $i - 1$ times is scored. After running all these simulations, they can be added together to obtain the total kerma.

The term “forced detection” (FD) is used in this work to refer to this technique, which has proven very useful in HVL and FAC correction factors calculations, and in the estimation of the scatter to CBCT scans. Other authors^{68–70} make use of this term for somewhat different techniques also for the estimation of the scatter contribution to CBCT scans.

2.2.7 Path length biasing (MFPTR)

A transformation of the probability distribution $p(\eta)$ of the number of mean free paths η to the next interaction can be used to increase the interactions deeper in a phantom (path stretching). This can be very valuable when the contribution from scattered particles to the kerma needs to be estimated. We have implemented a transformation for path length stretching which does not exhibit a dependency on the particle’s direction as is the case of the well known VRT *exponential transformation of the photon path length*.^{46,71} This dependency on the particle’s direction is a potential source of large weight fluctuations when large changes in particle’s direction arise.

2.2. USED VARIANCE REDUCTION TECHNIQUES (VRTS)

The transformation of $p(\eta)$ is chosen to be

$$p(\eta) = \frac{2 \cdot \eta_0^2}{(\eta + \eta_0)^3}, \quad (2.3)$$

with η_0 an adjustable parameter. This distribution shows an increased probability at larger η values and a decreased probability at small η values compared to the regular exponential distribution. To keep the game fair, the weight has to be modified accordingly to

$$wt' = wt \cdot \frac{0.5 \cdot e^{-\eta}}{\lambda \cdot \eta_0^2} \cdot (\eta + \eta_0)^3, \quad (2.4)$$

where λ is the photon mean free path. As can be seen, the weight of the photon does not depend on the direction of the particle which reduces the fluctuations of the weights and therefore has a reduced variance associated with it.

The number of mean-free-paths, η , is sampled from the probability density function (pdf) given by Eq. 2.3 using

$$\eta = \eta_0 \cdot \left(\frac{1}{\sqrt{1 - \xi}} - 1 \right), \quad (2.5)$$

with ξ a random number uniformly distributed between 0 and 1.

2.2.8 Woodcock tracing

Woodcock tracing³⁴ is a VRT also known as “delta scattering” or “fictitious interaction” method. It has been successfully used in electron transport to handle the energy-dependent cross sections.⁷² When applied to photon transport, photons are transported to the interaction site without checking geometrical boundaries, a very

time consuming operation in geometries with a large number of very small geometrical regions. To this end, a fictitious interaction is added to the possible interactions, which leaves the state of the particle unchanged. The cross-section for this interaction is selected in such a way that the total cross-section is constant in the entire geometry. For instance one can use the maximum cross-section $\mu_{max}(E)$ in the whole geometry as the constant value. A fictitious interaction with cross-section $\mu_{max}(E) - \mu_{ir}(E)$ is added to each region ir . Once at the interaction site, a possible photon interaction is selected among coherent scattering, incoherent scattering, photoelectric absorption or the fictitious interaction. In the case of the latter, particle energy and direction are left unchanged. This technique has been found to produce a 20% efficiency increase in xVMC⁴⁸ for photon beams in RT.

2.3 EGSnrc

This section describes EGSnrc, the MC simulation system, which is the calculation tool used for the work presented here. Section 2.3.1 gives a general overview of EGSnrc. Subsequent sections describe relevant EGSnrc features that have been added or modified during the course of this work.

2.3.1 General overview

The EGS (Electron Gamma Shower) system is a MC simulation toolkit for the coupled transport of electrons/positrons and photons in an arbitrary geometry for particles with energies above 1 keV up to several hundreds of GeV. The EGSnrc system,²² released in 2000, provides many improvements in the condensed history implementation of electron transport, better low-energy photon physics, more efficient sampling algorithms and several corrections to existing errors, compared to its predecessor EGS4.⁷²

EGSnrc has been extensively benchmarked in medical physics, and is therefore considered the “gold standard” in this field. A detailed description of this system and its capabilities can be found in the EGSnrc manual.⁷³

Users must write an user-code consisting of a main program, a scoring routine (historically called `ausgab`) and two subroutines that provide geometrical information to EGSnrc via a well defined interface. EGSnrc user-codes have been traditionally written in MORTRAN,⁷⁴ a FORTRAN-like language that is translated into FORTRAN by the MORTRAN pre-processor provided with the system. Starting with EGSnrc V4 (a.k.a EGSnrcMP),⁷⁵ EGSnrc’s multiplatform version, there is a C interface provided so that user-codes can be written in C or C++. EGSnrc is distributed with a series of MORTRAN user-codes for RZ and spherical geometries (`CAVRZnrc`, `CAVSPHnrc`, `DOSRZnrc`, `EDKnrc`, `FLURZnrc`, and `SPRRZnrc`) and C++ user-codes for the simulation of ionization chambers (`cavity`, `egs_chamber` and `egs_fac`). These user-codes are described in detail in the EGSnrc user-code manual.⁵⁶

Since 2005, the `egspp` EGSnrc C++ class library^{57,76} is distributed with EGSnrc, which provides a general purpose geometry package that can be used to model a wide range of geometrical structures, a set of most frequently used particles sources, base application classes for developing simple and advanced applications, a set of basic scoring classes, and other utility classes such as classes for sampling from a probability distribution, for handling system-dependent tasks (shared library loading, timing, etc.), for run control (parallel processing), a random number generator class, an alias table sampling class, a class for parsing input files, an interpolator class, among others.

The geometry module offers the possibility of simulating complex geometries in a very efficient fashion. Basic geometric objects such as planes, spheres, cylinders, cones, pyramids and prisms, with customized geometry checking algorithms, can be

combined into more complex objects (composite geometries) using logical relationships among them, optimized for speed. This functionality allows the definition of complex geometry by means of user input, *i.e.*, without having to resort to programming the geometry.

2.3.2 Interpolation accuracy of photon cross section data grid

All material data needed by EGS was initially generated with a stand-alone utility program called PEGS (Pre-processor for EGS) written in MORTRAN. With the release of EGS4, PEGS correspondingly became PEGS4, which is how this utility is still referred to. Currently, EGSnrc requires considerably more data than provided by PEGS4, which is read directly via the HATCH subroutine. For detailed information regarding the use of PEGS4, the reader is referred to the PEGS4 user's manual included in report PIRS-701, the EGSnrc manual.⁷³

Originally, the main field of application of EGS was high energy physics. For this reason, no attention was paid to the accuracy of the photon cross sections near atomic absorption edges⁷¹ and PEGS4 was designed to generate a grid with a maximum number of photon energy points (\$MXGE) in the entire energy range requested by the user. \$MXGE is a macro which sets the array dimensions for the energy-dependent photon data. Although \$MXGE can be changed in the PEGS4 code, PEGS4's algorithm for deciding how many bins to use might still pick many fewer bins than \$MXGE. The decision is based on the overall accuracy to reproduce the cross sections in the entire energy interval.

Typical PEGS4 data sets used in radiotherapy calculations are created for an energy range between 10 keV and 20 MeV. If these data sets are used in the

Figure 2.1: Mean free path λ for lead in the vicinity of the L1 and L2 atomic absorption edges for two different energy grids. Data sets generated by EGSnrc from the XCOM cross section compilation for an energy range 10 keV to 250 keV.

kilovoltage energy range, inaccuracies in the cross section interpolation procedure near absorption edges can potentially lead to errors in MC calculations. Figure 2.1 shows two cross section data sets for the same energy range (10 keV - 250 keV) when using different energy grids (200 and 2000 bins). A coarser energy grid will cause larger interpolation errors near the absorption edge.

A new capability has been added to EGSnrc which allows the use of any photon cross section raw data supplied by the user. The photon cross section from the PEGS4 data set is replaced on the fly, i.e., without the need to create an extra data file. First, one must create a PEGS4 data set for the desired energy interval, and then one specifies the name of the new cross section data file. Currently, EGSnrc offers such cross section data files for the XCOM⁷⁷ and EPDL97⁷⁸ compilations as al-

ternatives to the default cross sections (Storm and Israel⁷⁹). The XCOM compilation was developed at the National Institute of Standards and Technology (NIST) and is based on theoretical and experimental data. EPDL97 is part of the Lawrence Livermore National Laboratory (LLNL) Evaluated Nuclear Data Library. EPDL97 is also based on currently available photon data, experimental and theoretical. The same level of agreement is obtained for the calculations presented in this work when using either one of these compilations. To obtain the desired energy grid that minimizes the inaccuracies around absorption edges, one must change the number of interpolation points for the photon cross sections. This is achieved by replacing the macro \$MXGE with the desired number of interpolating points in any EGSnrc user code.

2.3.3 Electron impact ionization cross sections

Electron impact ionization (EII) is the process in which electrons or positrons interact with an atomic shell and create vacancies. Inner shell vacancies relax via the emission of characteristic x-rays, Auger and Coster-Kronig electrons. Since 2002, EGSnrc allows the creation of inner shell vacancies for all K- and L-shells with binding energies above 1 keV. Kawrakow⁸¹ developed a semi-empirical theory to calculate EII cross sections using a simplified generalized oscillator strength (GOS) function with the same properties as the Bethe surface. This model produces shell-wise differential electron inelastic scattering cross sections that reproduce the stopping power formula in its applicability range, describe measured inner shell EII cross sections well, are self-consistent and applicable to all shells. Cross sections obtained with this model are the default EII cross sections in EGSnrc. Figure 2.2 compares K-shell EII cross section data from various experiments with EGSnrc values and those of Casnati^{82,83} and Gryziński^{84–86} for copper and gold. Casnati’s semi-empirical fit to experimental data and the EGSnrc values reproduce the measurements similarly well, while Gryziński’s

Figure 2.2: Comparison of K-shell EII cross sections obtained from theoretical as well as empirical models with experimental data for copper and gold. Experimental data taken from Namito and Hirayama.⁸⁰

values underestimate them.

EII can be considered in EGS4 as an extension using the KEK low-energy package.⁸⁰ It is also available in other major MC codes such as MCNP,⁸⁷ ITS⁸⁸ and PENELOPE.⁸⁹ In the KEK low-energy implementation the user has the choice among several K-shell EII cross section compilations (Casnati, Jakoby,⁹⁰ Gryziński and Kolbenstvedt⁹¹). Casnati's cross section data are used as the default since they reproduce the measurements the best among the above mentioned compilations. The second choice is Gryziński's data since they are based solely on a theoretical model and can be used in energy regions where there are no experimental data. Figure 2.3 shows K-shell EII cross sections for tungsten according to these compilations together with the ones in EGSnrc. As one can see, Gryziński's semi-classical theory underestimates the EII cross sections compared to the values obtained by the other authors.

Figure 2.3: Available electron impact ionization cross sections for tungsten from different compilations. Only K-shell included in the graph.

EGSnrc has been modified to allow the use of arbitrary EII cross sections. One must first create a cross section data file with the proper format and indicate by input that a different EII cross section will be used. EII cross section data files for the K-shell with binding energies above 1 keV according to Casnati, Gryziński and Kolbenstvedt⁹¹ have been created and made available with the EGSnrc system. It is worth noticing that the default EII implementation in EGSnrc is not limited to the K-shell. These data files cover the energy range between the binding energy and 10 GeV for the first 100 elements of the periodic table.

2.3.4 Coherent scatter form factors.

Originally, the treatment of coherent (Rayleigh) scattering in EGSnrc was inherited from EGS4.⁷² In this approach the coherent scatter form factors for molecules are calculated from the independent atom approximation (IAA) by a weighted sum of atomic form factors.⁹² This is the default model in EGSnrc and many other general purpose MC codes. It is known to be inaccurate for small angle scattering because it does not take into account molecular interference effects. This can be seen in Fig. 2.4 where the coherent scattering cross-section in water for 25 keV photons has been calculated using the IAA (dashed line) and measured molecular form factors (solid line). These measured molecular form factors for coherent scattering are taken from the paper by Peplow and Verghese⁹³ for 15 materials. As of this writing, these data are available online at <http://www.ornl.gov/~5pe/p006.html> and are also distributed with EGSnrc. The treatment of the coherent process in EGSnrc is extended to allow the use of arbitrary photon coherent scatter form factors. In Chapter 6 the effect of molecular form factors for coherent scattering on the estimation of the scatter distribution from CBCT scans is studied.

In addition, an alias sampling algorithm for sampling coherent scattering an-

Figure 2.4: Coherent cross-sections for 25 keV photons in water calculated using the IAA (dashed line) and measured molecular form factors by Peplow and Verghese.⁹³

gles is implemented, which is more accurate for large angles than the original EGS4 implementation (see section 2.2.4 of PIRS-701 report⁹⁴). This has little effect on calculation results where Rayleigh scattering plays a role since the angular distribution for this interaction is predominantly forward peaked.

2.3.5 Incoherent scatter: norej option

The treatment of bound Compton scattering is extended in the EGSnrc system for the purposes of this investigation. In EGSnrc the total cross section resulting from the Klein-Nishina formula is used to compute total photon cross sections. The correct number of Compton interactions with bound electrons is recovered at run time by rejecting the appropriate amount of candidate Compton collisions. This implies that one cannot use the EGSnrc photon cross section interpolation tables directly

to remove the attenuation of the incident photon beam, and one must keep track of rejected Compton interactions. Although this is possible, the resulting scoring logic is very complex and prone to mistakes.

Thus, in the current EGSnrc version, one can request the use of the actual bound Compton total cross section in which case there are no rejected Compton interactions. To enable this option, the input key `Bound Compton scattering` in the `MC Transport Parameter` input section must be set to “`norej`” instead of “`on`” which is still left for compatibility with existing user-codes. With “`norej`”, rejections in subroutine `COMPT` lead to re-sampling rather than rejecting the entire interaction. This requires a new data file, `compton_sigma.data`, which contains the ratio of the bound Compton total cross section to the Klein-Nishina total cross section. This new implementation added a few optimizations that result in a 10% to 30% speed improvement, depending on energy and atomic number Z .

2.4 BEAMnrc

BEAMnrc^{28,95} is the most known and used EGSnrc user-code in medical physics. It was conceived under the OMEGA project, a collaboration between the NRC and the University of Wisconsin, with the purpose of developing a tool for simulating RT sources to develop 3-D treatment planning for RT. BEAMnrc has been widely used for the simulation of megavoltage medical linear accelerators. But it also provides an XTUBE component module that can be used to model x-ray tubes.

2.4.1 Kerma scoring with BEAMnrc

With BEAMnrc one can estimate the particle fluence $\phi(E)$ at user defined scoring planes. In the present work, the fluence scoring algorithm is extended to obtain the kerma at a scoring plane employing a user-supplied file of $E \cdot (\mu_{en}/\rho)$ values for the relevant media in the problem. If such a file is not provided, the mass energy transfer coefficient $E \cdot (\mu_{tr}/\rho)$ from the PEGS4 data sets is used instead. This constitutes a valid approximation at kilovoltage energies in air because the energy fraction lost to radiation is negligible. Another feature in BEAMnrc is the ability to calculate the dose deposited in any region defined as a dose scoring region in the input file.

Figure 2.5: Efficiency of a depth dose (kerma) calculation for a 160 kV x-ray beam in a water phantom for a Comet MXR-165 x-ray tube.

For the purposes of this investigation, the dose scoring algorithm is replaced with kerma scoring, based on a track-length estimator (see *e.g.* the work by Williamson⁹⁶ for a review on different methods for estimating kerma). With these additions, one can calculate kerma at scoring planes, inside defined volumes, or both. The availability of these estimation techniques can prove very useful in a variety of situations, where the kerma is needed. For example, Fig. 2.5 compares a kerma calculation in

a water phantom subjected to a 160 kV x-ray beam as a function of depth with and without track-length estimation. As can be seen, the track-length estimation technique is 20 times more efficient than the analog kerma calculation (scoring energy deposition every time a photon interacts).

Chapter 3

Efficient x-ray tube simulations with DBS

A proper characterization of the x-ray beam is crucial for the development and efficient use of an x-ray system. Experimental measurement of x-ray spectra requires special equipment only available in a limited number of laboratories. Since these measurements are time consuming and very difficult, different calculational approaches for estimating x-ray spectra have been developed. Semi-empirical^{97–100} and empirical models^{101–103} have been used to estimate the spectral x-ray distribution particularly in medical imaging simulations and dose calculations. Semi-empirical models make use of the Thomson-Whiddington relation to describe the penetration of electrons into a thick anode. This is a crude approximation that ignores backscatter and energy straggling.¹⁰⁴

An improved semi-empirical model was proposed by Poludniowski,^{104,105} which is based on a more realistic treatment of electron penetration using MC derived results as opposed to the semi-empirical treatment of the bremsstrahlung cross sections.

However, this model is based on several simplifying assumptions: isotropic x-ray emission and electron penetration depth in the anode which is much smaller than the focal spot size. Moreover, the characteristic spectrum is treated in a simple way, with no attenuation of the characteristic x-rays due to photoelectric absorption (indirect component) and an empirical model is used to take electron impact ionization (EII) into account. These simplifications could potentially have a significant effect on the accuracy of the predicted spectrum for applications such as mammography. This model requires running MC calculations to provide the joint probability density function describing the fraction of electrons as function of target depth with a given fraction of the initial energy. Although it offers an alternative to a full MC simulation for determining bremsstrahlung spectra for tungsten targets and targets of similar Z, it still suffers from similar limitations as previous semi-empirical models.

MC modeling remains the only alternative to overcome the above mentioned limitations. The availability of advanced MC simulation systems and the ever increasing computing power has made MC simulations of x-ray spectra an attractive addition and alternative to experimental measurements. As a consequence, the study and characterization of x-ray tubes using MC simulations has become common practice. Two major MC codes often used in medical physics are EGSnrc^{22,94} and MCNP4C.⁸⁷ Despite differences in their electron transport algorithms, these codes have achieved a similar level of maturity in the physics of photon and electron interaction cross sections.^{81,94,106} A study modeling complete x-ray units, including the target and tube voltage fluctuations, was published by Verhaegen *et al.*³¹ in 1999 using EGS4/BEAM.²⁸ That same year, Bhat *et al.*¹⁰⁷ published calculated off-axis x-ray spectra using EGS4.⁷² More recently, BEAMnrc²⁹ was used to generate x-ray spectra for a dosimetric and micro-dosimetric study of contrast-enhanced radiotherapy.¹⁰⁸ MCNP4C based simulations for modeling x-ray spectra in diagnostic radiology and mammography have been reported.^{30,32,109} Some authors have also employed ITS

3.0⁸⁸ to simulate x-ray spectra in mammography¹¹⁰ and radiosurgery x-ray tubes.¹¹¹ The MCNP package is often selected because of its powerful combinatorial geometry package. However, this generality and flexibility comes at the expense of an increase in calculation time as reported elsewhere in the literature.^{112–114}

Due to the small number of bremsstrahlung photons emitted by electrons in the keV energy range, x-ray tube MC simulations are very inefficient. This can be observed in Fig. 3.1 where the bremsstrahlung branching ratio $\sigma_{\text{brem}}/\sigma_{\text{tot}}$ is plotted as function of the electron energy for tungsten. Any gain in computation speed is therefore important when performing such simulations. The BEAMnrc^{28,29} EGSnrc user-code, more widely used for the simulation of megavoltage medical linear accelerators, provides an optimized geometry implementation that can be used to model x-ray tubes and was therefore selected for the purposes of this study. An investigation of the use of the recently developed general purpose EGSnrc geometry package,⁷⁶ which also could have been employed, is left for future publications.

Figure 3.1: Bremsstrahlung branching ratio for tungsten. Data generated with the `examin` user-code.

Ali and Rogers¹¹⁵ reported efficiency gains of about one order of magnitude when combining Bremsstrahlung Cross Section Enhancement (BCSE) with UBS or DBS compared to just using UBS or DBS especially for large fields of interest and 4π geometries. In this chapter the DBS efficiency, when applied to the simulation of x-ray machines for narrow beams, is investigated and compared to the efficiency of UBS simulations. A methodology for estimating the optimum splitting number is presented, which maximizes the calculation efficiency, saving a significant amount of computing time. Values of the DBS optimum splitting number for several practical situations involving x-ray tube simulations are reported.

3.1 X-ray tube simulations

At the National Research Council of Canada (NRC), medium energy x-ray beam qualities are obtained with a Comet MXR-320 bi-polar double-focal spot x-ray tube of advanced metal-ceramic design. The x-ray generating target is made out of tungsten and has an angle of 20° with a focal spot size of 3 mm by 3 mm. The x-ray beam is filtered with 3 mm of Be on its way out of the tube. Besides the lead and steel collimators of the shutter system, the experimental setup includes a lead block, which serves as shielding for personnel protection, and a beam defining lead diaphragm. For this study, beam qualities in this energy range were selected with an added filtration of 1 mm Al + 0.4954 mm Cu and tube potentials between 100 kV and 300 kV. A 160 kV beam from a Comet MXR-165 x-ray tube (30° target angle, 4 mm Be inherent filtration and 0.38 mm Cu added filtration), used for blood irradiation in North America, is also included in the efficiency study.

X-ray tube simulations are performed with the BEAMnrc^{28,29} user-code from the EGSnrc MC simulation system of photon and electron transport.^{22,94} The main

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Figure 3.2: BEAMnrc geometry used to model the Comet MXR-320 x-ray system with its collimation system. The x-ray target is modeled with the BEAMnrc component module XTUBE and the rest of the geometry with the component module FLATFILT.

component modules needed are XTUBE and FLATFILT (see the BEAMnrc manual²⁹ for details on these modules). Figure 3.2 shows the BEAMnrc geometry used to model the COMET MXR-320 x-ray tube with the collimation system used at NRC. Electrons and photons are followed down to a threshold energy of 1 keV, which is the lowest transport energy available in the EGSnrc system. However, due to the added Al and Cu filtration, no photon with energy below 10 keV reaches the scoring field for the medium energy x-ray beams, hence a photon transport cut-off energy (PCUT) of 10 keV is used in this energy range. The scoring field is a user-defined circle where the

3.1. X-RAY TUBE SIMULATIONS

quantity of interest such as the air-kerma or the particle fluence is scored.

Binding effects and Doppler broadening are taken into account in the simulation of Compton scattering. EII according to the approach by Kawrakow⁸¹ and the relaxation cascade of inner shell vacancies created in photo-absorption are turned on. Rayleigh scattering is also included in the calculations. The best cross-sections available with EGSnrc are used in all simulations: the NIST tabulations of differential bremsstrahlung cross sections,^{116,117} which are the basis for the ICRU-37¹¹⁸ recommended radiative stopping powers, and photo-absorption and Rayleigh scattering total cross sections from the XCOM¹¹⁹ tabulations. Simple angular bremsstrahlung sampling is used in order to take full advantage of the DBS algorithm. In this case only the leading term of the Koch-Motz angular distribution is used for sampling the bremsstrahlung photon direction.

To save computing time, range rejection is set globally for total electron energies below 1 MeV. Calculations at 50 keV and 200 keV for a DBS splitting number of 10000 with and without range rejection show no difference in the kerma or fluence results within 2% one sigma uncertainty. At the same time, calculation times are significantly longer without range rejection, ranging between a factor of 2 longer at 50 kV and a factor of 5 longer at 200 kV.

3.2 Efficiency of photon fluence calculations.

A rigorous theoretical explanation of the efficiency dependency of DBS and UBS simulations on the splitting number N was given by Kawrakow.¹²⁰ According to the results of that paper, the efficiency ε_N is given by

$$\varepsilon_N^{DBS} = \frac{\varepsilon N}{[1 + \alpha\beta(N - 1)][1 + cA(N - 1)]} \quad (3.1)$$

3.2. EFFICIENCY OF PHOTON FLUENCE CALCULATIONS.

where ε is the efficiency without splitting and α is the average probability that a primary electron undergoing a bremsstrahlung event produces a photon going towards the field of interest. Here, β is the ratio of the average time per shower to transport bremsstrahlung photons and all their descendants (electrons and photons) to the average total time per shower, and the product cA is the probability that a photon reaches the scoring zone of area A . To obtain the expression for the efficiency of UBS, ε_N^{UBS} , one only has to substitute the product $\alpha\beta$ in Eq. (3.1) with β .

The optimum splitting number N_{max}^{DBS} , which maximizes the efficiency of a photon fluence simulation given a scoring zone area A , can be derived¹²⁰ from Eq. (3.1). This optimum splitting number is given by the expression

$$N_{max}^{DBS} \approx \frac{1}{\sqrt{\alpha\beta cA}} \quad (3.2)$$

since the probability of a bremsstrahlung photon reaching the scoring plane cA is very small and $\beta \ll 1$.

Rearranging Eq. (3.1) into a second order polynomial expression for N/ε^{DBS} as a function of $N - 1$ one obtains

$$\frac{N}{\varepsilon_N^{DBS}} = A_0 + A_1(N - 1) + A_2(N - 1)^2 \quad (3.3)$$

where the polynomial coefficients A_i are defined as follows

$$\begin{aligned} A_0 &= \frac{1}{\varepsilon} \\ A_1 &= \frac{\alpha\beta + cA}{\varepsilon} \\ A_2 &= \frac{\alpha\beta cA}{\varepsilon} \end{aligned} \quad (3.4)$$

One can practically determine the optimum splitting number N_{max}^{DBS} by calculating the

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quantity of interest, in this case the photon fluence or any photon fluence dependent quantity such as kerma, for a few different splitting numbers N . The efficiencies ε_N^{DBS} are computed from the uncertainties and the CPU times for these calculations. A simple quadratic fit to the ratio N/ε_N^{DBS} as function of $N - 1$ provides the polynomial coefficients A_i . Using equations (3.2) and (3.4), the optimum splitting number N_{max}^{DBS} can be calculated as

$$N_{max}^{DBS} \approx \frac{1}{\sqrt{\alpha\beta cA}} = \sqrt{\frac{A_0}{A_2}} \quad (3.5)$$

and the relative efficiency gain of DBS over an analog calculation can be obtained from equations (3.3) and (3.4)

$$\frac{\varepsilon_N^{DBS}}{\varepsilon} = \frac{A_0 N}{A_0 + A_1(N - 1) + A_2(N - 1)^2} . \quad (3.6)$$

The methodology described above is used to find the optimum splitting number N_{max}^{DBS} for air-kerma calculations at 1 m from the x-ray target on a 5 mm radius scoring field. This setup corresponds to the actual diaphragm opening of a free air chamber (FAC) in use at NRC for HVL measurements. Since these measurements are corrected for attenuation and scatter, a DBS splitting radius²³ equal to the scoring field radius is chosen.

3.3 Optimum efficiency gain for kilovoltage beams.

The efficiency gain due to DBS for kilovoltage beams is expected to be larger than the efficiency gain observed in the megavoltage case.¹²⁰ This observation can be explained by the fact that, in the kilovoltage case, there are fewer photons per incident electron and therefore β is much smaller, and the fact that the angular distribution of bremsstrahlung emission is much more uniform and therefore the average probability

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for a photon to be emitted towards the scoring area, $\langle p \rangle$, is much smaller. Hence, the maximum efficiency gain of using DBS over not using splitting at all, would be given by the inverse of $\langle p \rangle$ ¹²⁰

$$\frac{\varepsilon_{max}^{DBS}}{\varepsilon} \approx \frac{1}{\langle p \rangle} = \frac{1}{cA} . \quad (3.7)$$

The probability $\langle p \rangle$ can be separated into the average probability of bremsstrahlung photons being emitted into the scoring area, $\langle \eta \rangle$, and the average probability $\langle \nu \rangle$ of these photons to reach the scoring area without being attenuated along their path. For a monoenergetic photon beam of energy E , the probability ν for a photon not being attenuated when passing through media with linear attenuation coefficients μ_i and thicknesses t_i is given by

$$\nu = e^{-\sum \mu_i(E) \cdot t_i} . \quad (3.8)$$

The average probability $\langle \nu \rangle$ for a spectrum $\phi(E)$ at the scoring plane is then

$$\langle \nu \rangle = \frac{\int \phi(E) \cdot e^{-\sum \mu_i(E) \cdot t_i} dE}{\int \phi(E) dE} . \quad (3.9)$$

The probability $\langle \eta \rangle$ for bremsstrahlung emission into the scoring area A can not be calculated analytically in the general case. However, for nearly uniformly distributed emission angles one has $\langle \eta \rangle \approx A/(4\pi d^2)$ and therefore

$$\frac{\varepsilon_{max}^{DBS}}{\varepsilon} = \frac{4\pi d^2}{A} \frac{\int \phi(E) dE}{\int \phi(E) \cdot e^{-\sum \mu_i(E) \cdot t_i} dE} \quad (3.10)$$

with d denoting the distance between the bremsstrahlung target and the scoring plane. For instance, for $A = 1 \text{ cm}^2$ and $d = 100 \text{ cm}$, one can expect an efficiency gain of more than a factor of 10^5 compared to a simulation without splitting!

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3.4 Results and Discussion

To minimize the uncertainty one is always interested in large production runs. The optimum DBS splitting number provides the best compromise between CPU time and statistical uncertainty. As mentioned in section 6.1, the optimum splitting number for DBS, N_{max}^{DBS} , can be determined by running several calculations with different splitting numbers and fitting a second order polynomial to the ratio of the splitting number to the calculation efficiency according to Eq. (3.3). As an example, Fig. 3.3 shows the determination of N_{max}^{DBS} for the 135 kV beam from the Comet MXR-320 x-ray unit installed at NRC. It is worth noting the good agreement between the theory (i.e., the quadratic form) and the MC results. Similar levels of agreement are observed for x-ray beam qualities of 150 kV and 200 kV.

A further test of the validity of the theory is to compare the actual efficiency of a MC calculation without splitting and the efficiency extracted from the quadratic fit as the inverse of A_0 , according to Eq. (3.4). To perform this comparison, the air-kerma is calculated for a 5 mm radius circular field at 1 m from the target of a Comet MXR-320 unit operated at 200 kV using a simulation without splitting. The statistical uncertainty is 13% after simulating 10^9 incident electrons. The corresponding CPU time is 70.85 hours resulting in an efficiency of $2.32 \times 10^{-8} \text{s}^{-1}$. The no-splitting efficiency calculated from the coefficient A_0 obtained from the fit of the DBS efficiency is $2.28 \times 10^{-8} \text{s}^{-1}$ thus confirming the validity of the theoretical expression given in Eq. (3.1).

3.4.1 Optimum splitting number and maximum efficiency

While the optimum splitting number for a 135 kV beam is about 7.6×10^5 , for higher energies this number decreases. A similar efficiency study shows that for 150 kV and

Figure 3.3: $N_{\text{max}}^{\text{DBS}}$ estimation for a Comet MXR-320 at 135 kV tube potential based on several MC calculations for 8 different splitting numbers. To measure efficiency, the relative statistical uncertainty in the air-kerma is used.

200 kV beams, the optimum splitting numbers are about 6.1×10^5 and 3.7×10^5 respectively. With increasing electron energy, the probability for emitting bremsstrahlung photons per incident electron increases. Therefore, more bremsstrahlung photons will be directly generated, thus effectively producing a similar number of photons on the scoring zone with a smaller splitting number.

A second observation from Fig. 3.3 is the magnitude of $N_{\text{max}}^{\text{DBS}}$. For megavoltage linac beams, Kawrakow *et al.*²³ reported optimum splitting numbers of up to 2.5×10^3 for a 6 MV $10 \times 10 \text{ cm}^2$ beam. The present study shows that for kilovoltage x-ray beams $N_{\text{max}}^{\text{DBS}}$ is significantly higher. For small scoring fields (5 mm radius circular field), necessary *e.g.* in the case of HVL calculations, $N_{\text{max}}^{\text{DBS}}$ can be as much as 2 orders

3.4. RESULTS AND DISCUSSION

of magnitude larger than in the megavoltage case. However, N_{max}^{DBS} depends strongly on the specific setup and beam characteristics. For instance, when simulating a 160 kV beam from a Comet MXR-165 x-ray tube (30° target angle, 4 mm Be inherent filtration and 0.38 mm Cu added filtration), used for blood irradiation in North America, N_{max}^{DBS} is only 1.7×10^4 for a kerma calculation in a 7.5 cm radius water phantom, but 1.04×10^6 for a HVL calculation of the same beam. The methodology presented here is therefore very useful for practical x-ray simulations as it permits the easy and quick determination of N_{max}^{DBS} for the situations of interest.

Figure 3.4: Relative efficiency gain of the DBS splitting technique for three kilovoltage beam qualities from a Comet MXR-320 x-ray system. Efficiency here is for air-kerma scoring at 1 m on a 0.5 cm radius field.

Once the polynomial coefficients A_i are known, one can use Eq. (3.6) to calculate the relative efficiency gain as a function of the splitting number. This is

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illustrated in Fig. 3.4 for the 135 kV, 150 kV and 200 kV beams from the Comet MXR-320 x-ray unit. Up to 5 orders of magnitude efficiency gain can be obtained using DBS over not using a splitting technique, reflecting the inefficiency of the bremsstrahlung production and the small scoring field. At higher energies, the presence of more bremsstrahlung photons limits the splitting efficiency gain since the bremsstrahlung production itself is already more efficient. In that case, the balance between the efficiency gain due to a reduction in the variance and the negative effect of the CPU time increase is reached at lower splitting numbers.

One conclusion that can be drawn from Eq. (3.2) is that N_{max}^{DBS} increases roughly as $1/\sqrt{A}$. As a consequence, if one increases the scoring radius by a factor of 2, then N_{max}^{DBS} is expected to decrease by roughly half the value for the smaller field as shown in Fig. 3.5. While the optimum splitting number N_{max}^{DBS} for a 1.0 cm radius scoring field is 4.1×10^5 , N_{max}^{DBS} is about 1×10^6 for a 0.5 cm radius scoring field.

3.4.2 DBS *versus* UBS.

UBS was the only bremsstrahlung splitting technique previously available for x-ray tube simulations with BEAM or BEAMnrc. An efficiency study to compare DBS with UBS is performed for a 160 kV beam from the Comet MXR-165 x-tube mentioned in section 3.4.1. Figure 3.6 shows the relative efficiency gain for DBS and UBS as a function of the splitting number. The maximum efficiency gain is 4.82×10^3 at $N_{max}^{UBS} = 7.17 \times 10^4$ for UBS, and 2.88×10^5 at $N_{max}^{DBS} = 1.04 \times 10^6$ for DBS. This implies that modeling x-ray tubes using DBS is 60 times more efficient than using UBS, if optimum splitting numbers are employed for both techniques.

From this study, one can evaluate the efficiency gain for a given splitting number. If one uses UBS with the recommended bremsstrahlung splitting number for linac

Figure 3.5: Relative efficiency gain of the DBS splitting technique for two scoring fields. Simulation of a Comet MXR-165 x-ray beam at 160 kV tube potential on small detector of 1 mm thickness at 1 m.

simulations of 100, as was done in previous publications using BEAM and BEAMnrc, then employing DBS with the optimum splitting number is about 2800 times more efficient. To put this into perspective, the simulations reported by Verhaegen *et al.*³¹ which took days to complete, could be done in less than a minute today, and not more than a few minutes with the computing power available at the time of publication of their paper.

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Figure 3.6: Relative kerma efficiency gain comparison between the DBS and UBS splitting techniques for a Comet MXR-165 x-ray tube. A 160 kV x-ray beam, incident on a 5 mm radius circular field at 1 m from the target is simulated. When using the optimum splitting number for both splitting techniques, DBS is 60 times more efficient than UBS.

3.4.3 Efficiency gain at low x-ray energies.

The emission of bremsstrahlung photons becomes more isotropic with decreasing electron energy. As a consequence, for sufficiently low energies, the average probability for emitting bremsstrahlung photons into the scoring field, $\langle\eta\rangle$, should be approaching $\langle\eta\rangle = A/(4\pi d^2)$ as discussed in section 3.3. To test this assumption, the maximum efficiency gain $\epsilon_{\text{max}}^{\text{DBS}}/\epsilon$ and the average attenuation $\langle\nu\rangle$ are calculated for a spectrum of 50 kV x-ray photons incident on a 0.5 cm radius scoring field at 100 cm from the target, corresponding to $\langle\eta\rangle = 0.625 \times 10^{-5}$.

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Figure 3.7: Relative efficiency gain of a fluence calculation for a Comet MXR-320 x-ray tube at 50 kV tube potential using the DBS splitting technique. Scoring is done on a circular field of 5 mm radius at 1 m from the source.

Figure 3.7 shows the whole efficiency gain curve as a function of the splitting number for the MC values (open squares) and the second order polynomial expression (line). The maximum efficiency gain $\epsilon_{max}^{DBS} / \epsilon$ is 1.603×10^6 (solid square) at a splitting number of 5.627×10^6 . This efficiency gain is one order of magnitude higher than the efficiency gains reported at higher energies in the previous section. As one can observe, this curve is relatively flat around the maximum efficiency gain. Since the maximum splitting number one can use in a simulation is limited by the computer memory, one can employ smaller splitting numbers with relatively little impact on the calculation efficiency.

The inverse of the maximum efficiency gain value is 0.624×10^{-6} . Therefore, for

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a completely isotropic bremsstrahlung emission, the average attenuation $\langle \nu \rangle$ should be approximately 0.1 in order to explain the observed efficiency gain. To find the actual $\langle \nu \rangle$, a spectrum at the scoring plane is obtained and processed by a simple FORTRAN program to evaluate expression (3.9) on page 39. The calculated $\langle \nu \rangle$ value is found to be 0.106, i.e., only 6% different from the value expected for an isotropic bremsstrahlung emission. Hence, within 6%, isotropic bremsstrahlung emission and the resulting Eq. (3.10) can be used to calculate the maximum efficiency gain for such low energy x-rays.

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Chapter 4

Free-air chamber correction factors

The best instrument for the absolute measurement of air-kerma at x-ray beam qualities below 500 kV is the free-air chamber (FAC). For this reason, they are used as the standard against which other x-ray detectors are calibrated. A FAC is a parallel-plate ionization chamber with air walls, ideally thick enough to establish charged particle equilibrium (CPE) in the collecting volume. Mostly, a system of parallel plates (a high potential plate opposite to a guard plate onto which the collector plate has been mounted in the center) is surrounded by aluminum guard bars to make the electric field uniform and perpendicular to the collector. These plates must be separated far enough to keep the loss of electron energy to a an acceptable minimum. The mass of air from which the electrons are released by photon interactions must be accurately known. The volume of this mass of air is defined by the effective area of the entrant aperture and by the edges of the collecting plate. Contribution to the ionization in the collecting volume by photons scattered out of the beam should be kept as low as possible. To avoid the effect of stray radiation, adequate shielding is provided by a box lined with lead sheets.

Since it is impossible to completely satisfy the above requirements in practice,

the FAC signal reading (corrected for humidity, temperature, pressure, ion recombination, polarity effect, and electrometer accuracy) must be corrected for several effects before it can be related to the air-kerma at the point of measurement (POM), i.e., the position of the beam limiting diaphragm. Typically, these corrections account for scatter contribution to the signal, signal reduction due to electron-loss from the collecting volume and attenuation of the photon beam along the path from the POM to the center of the sensitive volume. While such correction factors have been determined experimentally in the past,^{121–123} measuring some of them directly involves taking the FAC apart, thus modifying the primary standard. This is the case for the corrections accounting for photon scatter and electron-loss. Therefore, several authors^{124–126} have proposed to estimate these two correction factors by means of MC simulation. The correction for attenuation, which is particularly important in the soft x-ray region, is still obtained experimentally using an evacuated-tube technique (*e.g.* employed at NRC) or a variable-pressure tube technique (used *e.g.* at BIPM) among other techniques.

Previous MC investigations of FAC correction factors suffer from two limitations. First, the combination of MC computed correction factors for photon scatter and electron loss with a measured correction for attenuation is not self-consistent, as shown by Mainegra-Hing *et al.*¹²⁷ using a simple model. The simple example considered in that paper demonstrates that an experimental correction that removes the effect of photon attenuation due to an air slab of thickness $L + h/2$, as in the evacuated-tube technique, does not completely correct for the effect, and that the lack of CPE along the beam direction can not be completely ignored. Although both effects are small in practice, it is unsatisfactory to rely upon a non self-consistent set of correction factors in a primary standard. Second, all investigations use simplifications in the incident beam and in the chamber geometry.

The purpose of this chapter is to introduce a self-consistent set of FAC correction factors (section 4.1) and to present their calculation by means of MC simulations that combine a complete simulation of the x-ray tube with a realistic model of the FAC geometry (section 4.4). Comparisons between computed and measured correction factors for the National Research Council of Canada primary standard in the medium x-ray energy range, where measured corrections are believed to be accurate, are given in section 4.5. FAC correction factors for the low x-ray energy range are presented in section 4.6 for lightly filtered beam qualities and mammography beam qualities (molybdenum filtration). A detailed analysis of the uncertainties arising from the uncertainties in the cross sections used in the simulations, is left for future work.

4.1 Formal derivation and definition of correction factors

The FAC signal reading can be related to the air collision kerma , K_{col} , at the point of measurement (POM), defined at the back of the beam limiting aperture, using

$$\frac{Q}{m} \left(\frac{W}{e} \right) = A_{\text{tot}} K_{\text{col}} , \quad (4.1)$$

with Q denoting the charge measured by the FAC (corrected for humidity, temperature, pressure, ion recombination, polarity effect, and electrometer accuracy) , and (W/e) the average energy needed to produce an ion pair in dry air.

The correction A_{tot} is obtained from a self-consistent set of correction factors as introduced by Mainegra-Hing *et al.*¹²⁷ using

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$$A_{\text{tot}} = A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_{\text{g}} A_{\text{att}} A_{\text{b}} . \quad (4.2)$$

A formal derivation of these corrections starts by relating the measured charge in the collecting volume (CV) of the FAC, Q , with the energy deposited in the CV, ΔE_{g} :

$$Q \left(\frac{W}{e} \right) = \Delta E_{\text{g}} . \quad (4.3)$$

The right-hand-side (rhs) of Eq. (4.3) is multiplied and divided by ΔE_1 , which is the energy that would be deposited in the CV of the FAC if the field defining aperture was totally absorbing:

$$Q \left(\frac{W}{e} \right) = \frac{\Delta E_{\text{g}}}{\Delta E_1} \Delta E_1 \equiv A_{\text{ap}} \Delta E_1 . \quad (4.4)$$

The above equation defines the correction factor A_{ap} needed to correct for leakage and scatter from the FAC aperture. The next step in the derivation is to multiply and divide the rhs of the above equation with ΔE_2 , the energy that would be deposited in the CV of the FAC if there were no contributions from secondary photons interacting in the air. Here, “secondary photons” means Compton or Rayleigh scattered photons, bremsstrahlung photons generated by the slowing down electrons, and fluorescent photons from the relaxation of shell vacancies created by photon or electron impact. The ratio $\Delta E_1/\Delta E_2$ can be identified with A_{scat} , the factor correcting for photon scatter:

$$Q \left(\frac{W}{e} \right) = A_{\text{ap}} \frac{\Delta E_1}{\Delta E_2} \Delta E_2 \equiv A_{\text{ap}} A_{\text{scat}} \Delta E_2 . \quad (4.5)$$

Note that our definition of A_{scat} differs from Burns¹²⁸ who uses separate correction factors for scattered photons and fluorescent photons, *i.e.*, our A_{scat} is the same as Burns’ $A_{\text{scat}} A_{\text{fl}}$. One can proceed by multiplying and dividing the rhs of the last

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equation with ΔE_3 ,

$$\Delta E_3 = \Delta E_2 + \Delta E_{\text{side}}. \quad (4.6)$$

Here, ΔE_{side} is the difference between the energy of primary electrons leaving and entering the cavity through the side faces of the CV. Here and in what follows the term “primary electrons” is used to denote the electrons set in motion by photons that have not interacted yet and have not visited a region identified as aperture. The ratio $\Delta E_2/\Delta E_3$ corrects for energy lost through the side faces of the CV and should therefore be defined as the electron loss correction A_{eloss} ,

$$Q \left(\frac{W}{e} \right) = A_{\text{ap}} A_{\text{scat}} \frac{\Delta E_2}{\Delta E_3} \Delta E_3 \equiv A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} \Delta E_3. \quad (4.7)$$

The rhs of the above equation is now multiplied and divided by ΔE_4 ,

$$\Delta E_4 = \Delta E_3 + \Delta E_{\text{FB}}, \quad (4.8)$$

where ΔE_{FB} denotes the difference between the energy of primary electrons leaving and entering the cavity through the front and back faces of the CV. If CPE along the beam direction existed, one would have $\Delta E_{\text{FB}} \equiv 0$. The ratio $\Delta E_3/\Delta E_4$ can therefore be identified as a CPE correction, *i.e.*,

$$Q \left(\frac{W}{e} \right) = A_{\text{ap}} A_{\text{scat}} A_{\text{att}} \frac{\Delta E_3}{\Delta E_4} \Delta E_4 \equiv A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} \Delta E_4. \quad (4.9)$$

Note that the imbalance between primary electrons entering and leaving the CV has been completely removed in ΔE_4 . Thus, ΔE_4 can be computed assuming that electrons deposit their energy, excluding the energy lost to radiation, locally on the spot. If there are $\psi(E, x, y, u, \phi)$ photons with energy E and position x, y passing through the aperture opening traveling at polar and azimuthal angles θ and ϕ with

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respect to the opening normal ($u = \cos \theta$), ΔE_4 is given by

$$\begin{aligned} \Delta E_4 = & \int dE \int dx dy \int du d\phi \psi(E, x, y, u, \phi) E \mu_{\text{en}}(E) \\ & \times \frac{1}{\mu(E)} \left[\exp\left(-\mu(E) \frac{L}{u}\right) - \exp\left(-\mu(E) \frac{L + us(x, y, u, \phi)}{u}\right) \right] \end{aligned} \quad (4.10)$$

Here, $\mu(E)$ and $\mu_{\text{en}}(E)$ are the linear air attenuation and energy absorption coefficients for photons with energy E , L is the distance from the point of measurement plane to the front of the CV, and $s(x, y, u, \phi)$ is the path length through the CV of the FAC for x, y, u, ϕ . The factor in the square brackets divided by $\mu(E)$ arises from the integration of $\exp(-\mu(E)t)$, which is the attenuation of the photon beam at a distance t from the point of measurement, for t between L/u and $L/u + s(x, y, u, \phi)$. The integration over x and y is limited to the aperture opening, which has a radius R , *i.e.* $x^2 + y^2 < R^2$. We now multiply and divide Eq. (4.9) with ΔE_5 ,

$$\begin{aligned} \Delta E_5 = & \int dE \int dx dy \int du d\phi \psi(E, x, y, u, \phi) E \mu_{\text{en}}(E) \\ & \times \frac{1}{\mu(E)} \left[\exp\left(-\mu(E) \frac{L}{u}\right) - \exp\left(-\mu(E) \frac{L + h}{u}\right) \right], \end{aligned} \quad (4.11)$$

where the only difference between ΔE_4 and ΔE_5 is that $s(x, y, u, \phi)$ has been replaced with h/u with h denoting the cavity height. If the incident beam was a parallel beam or a point source, ΔE_4 would be equal to ΔE_5 . The ratio $\Delta E_4/\Delta E_5$ therefore accounts for the actual geometry of the beam (finite spot size, scatter in the air before (up-stream) the aperture, off-focal radiation from the x-ray tube, etc.) and is thus defined as a geometry correction factor A_g :

$$Q\left(\frac{W}{e}\right) = A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} \frac{\Delta E_4}{\Delta E_5} \Delta E_5 \equiv A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_g \Delta E_5. \quad (4.12)$$

The next step is to multiply and divide Eq. (4.12) with ΔE_6 , the energy that would

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be deposited if the ideal photon beam was not attenuated,

$$\Delta E_6 = \int dE \int dx dy \int du d\phi \psi(E, x, y, u, \phi) \frac{h}{u} E \mu_{\text{en}}(E) , \quad (4.13)$$

and to identify $\Delta E_5/\Delta E_6$ with the attenuation correction A_{att} , *i.e.*,

$$Q \left(\frac{W}{e} \right) = A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_{\text{g}} \frac{\Delta E_5}{\Delta E_6} \Delta E_6 \equiv A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_{\text{g}} A_{\text{att}} \Delta E_6 . \quad (4.14)$$

We now note that

$$\Delta E_6 = K'_{\text{col}} \pi R^2 h \rho \equiv K'_{\text{col}} m \quad (4.15)$$

where ρ is the mass density of air, m the mass of air in a cylinder with radius R and height h , and K'_{col} is the average collision air kerma with the aperture present but totally absorbing (average means averaged over the circle defined by the aperture opening). Using the above equation in Eq. (4.14) one has

$$\frac{Q}{m} \left(\frac{W}{e} \right) = A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_{\text{g}} A_{\text{att}} K'_{\text{col}} \quad (4.16)$$

The final step in the derivation is to multiply and divide the rhs of the above equation with K_{col} , the air collision kerma at the location of the aperture with the FAC removed,

$$\frac{Q}{m} \left(\frac{W}{e} \right) = A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_{\text{g}} A_{\text{att}} \frac{K'_{\text{col}}}{K_{\text{col}}} K_{\text{col}} \equiv A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_{\text{g}} A_{\text{att}} A_{\text{b}} K_{\text{col}} \quad (4.17)$$

thus relating K_{col} , the quantity being measured, to the charge Q collected in the FAC. The correction factor $A_{\text{b}} \equiv K'_{\text{col}}/K_{\text{col}}$ accounts for photons backscattering in air towards the measurement point, which are not present when the FAC is in place and the aperture is totally absorbing. One can expect that this correction will be

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very small, but it is included for the sake of a completely rigorous derivation.

The correction factors A_g , A_b and A_{cpe} are neglected in existing primary FAC standards. In sections 4.5 and 4.6 A_g and A_{cpe} are shown to be very small. However, A_b , the correction for photon backscattering into the scoring field, becomes non-negligible for low-energy x-ray beams and should be taken into account. The correction factor A_{ap} is ignored in the NRC standard, although McEwan,¹²⁹ Grimbergen *et al.*,¹²⁴ and Kurosawa and Takata¹³⁰ have pointed out the need to take into account photons leaking through, or bouncing off, the aperture diaphragm to enter the FAC. The definitions of A_{scat} and A_{eloss} given here are consistent with previous MC calculations of these factors^{124–126,128} (except that Burns¹²⁸ splits A_{scat} into separate scatter and fluorescence corrections). The use of a computed instead of a measured attenuation correction therefore represents the most significant departure from previous work. The advantage of using a calculated A_{att} is that the small inconsistency noted in Ref.¹²⁷ is removed. The main drawback of a computed attenuation correction is that A_{att} will depend on the details of the photon spectrum impinging on the FAC and on the photon interaction cross sections employed in the simulations, thus potentially increasing its uncertainty. One practical way of dealing with this issue is to multiply and divide Eq. (4.17) with A'_{att} , where A'_{att} is the MC computed attenuation correction corresponding to the experimental procedure used to determine A_{att} . For instance, for the evacuated-tube technique employed at NRC,

$$A'_{att} = \frac{\Delta E'_g}{\Delta E''_g} \quad (4.18)$$

where $\Delta E'_g$ and $\Delta E''_g$ are the energies deposited in the CV when a brass tube of length $L + h/2$ with Be windows, filled with air ($\Delta E'_g$) or vacuum ($\Delta E''_g$), is inserted between the x-ray tube and the FAC aperture. The difference between A_{att} and A'_{att} accounts for the inconsistency of this technique noted in Ref.¹²⁷ and also for changes in the

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photon spectrum due to attenuation and scatter caused by the presence of the tube. Both effects are very small in practice so that A_x ,

$$A_x = \frac{A_{\text{att}}}{A'_{\text{att}}} , \quad (4.19)$$

will be very close to unity. As a result, even large uncertainties in the incident photon spectrum and/or attenuation coefficient will translate into a very small uncertainty in A_x . With this additional correction factor, Eq. (4.17) reads

$$\frac{Q}{m} \left(\frac{W}{e} \right) = A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_g A_x A'_{\text{att}} A_b K_{\text{col}} . \quad (4.20)$$

One can now replace A'_{att} in the above equation (but not in the definition of A_x) with the measured attenuation correction $A_{\text{att,exp}}$ to arrive at

$$\frac{Q}{m} \left(\frac{W}{e} \right) = A_{\text{ap}} A_{\text{scat}} A_{\text{eloss}} A_{\text{cpe}} A_g A_x A_{\text{att,exp}} A_b K_{\text{col}} . \quad (4.21)$$

The disadvantage of this approach is that it requires the calculation of dose deposited in the CV in three different geometries to obtain A_x .

Equation (4.17) offers a comprehensive set of corrections for the determination of the air collision kerma from experimental FAC measurements. If measured values of $A_{\text{att,exp}}$ are available, one can use Eq. (4.21) to correct the FAC signal as long as any inconsistency in the experimental procedure can be accounted for through a determination of A_x . The implementation details on how to calculate these correction factors are given in the next section.

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4.2 Calculation of correction factors using MC simulations

The EGSnrc system^{22,94} is selected as the MC simulation toolkit due to its proven ability to perform ionization chamber calculations^{131,132} with high accuracy and self-consistency. Starting from the EGSnrc C++ code `cavity`,⁷⁶ a new C++ EGSnrc user-code, called `egs_fac` in what follows, is developed. The `cavity` code has the ability to perform the simulation of the transport of the same source particle through different geometries. This functionality is kept in `egs_fac` so that one can obtain A_x in a single simulation. As explained in section 2.3.5 of Chapter 2, the actual bound Compton total cross section is used and there are no rejected Compton interactions.

In order to be able to calculate the various deposited energies ΔE_i , $i = \text{g, side, FB, } 1 \dots 6$, two extra properties are maintained during the simulation for all particles (in addition to charge, energy, position, etc.). These extra properties will be denoted as l and κ in the following (in practice l is stored in the EGSnrc LATCH variable⁹⁴ whereas κ is maintained in an additional array added to the particle stack). Note that κ is only needed for an algorithm that improves the efficiency of the calculation of A_{cpe} discussed below. In addition, the user defines “side” and “front/back” regions adjacent to the CV in the `egs_fac` input file. The particle properties l and κ are set and modified as follows during the simulation:

- For particles obtained from the radiation source, l is set to 0 and κ to 1.
- Particles with $l = 0$ hitting any aperture region are given $l = -1$
- Secondary particles created in photon and electron interactions inherit l and κ from the incident particle, except for modifications noted below, which only apply to interactions occurring downstream of the POM.

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- When an $l = 0$ photon undergoes an interaction all resulting scattered photons are set to $l = 1$.
- All bremsstrahlung photons from $l = 0$ electrons are set to $l = 1$
- All fluorescent photons are set to $l = 1$, provided the particle that created the inner shell vacancy (photons in photo-absorption or bound Compton scattering, and electrons in impact ionization) had $l = 0$.
- After each $l = 0$ photon step, κ is multiplied by $\exp(\lambda)$, where λ is the number of mean-free paths traveled by the photon during the step.

The above set of rules makes it possible to distinguish between energy deposition events from primary or scattered particles as well as to undo the effect of photon attenuation. The various energies $\Delta E_i, i = \text{g, side, FB}, 1 \dots 6$ needed for the correction factors are obtained as follows:

$\Delta E_g = \text{Sum of all CV energy depositions}$

$\Delta E_1 = \text{Sum of } l \geq 0 \text{ CV energy depositions}$

$\Delta E_2 = \text{Sum of } l = 0 \text{ CV energy depositions}$

$\Delta E_{\text{side}} = \text{Difference between the energy of } l = 0 \text{ electrons entering}$
 and leaving the CV through the side faces

$\Delta E_{\text{FB}} = \text{Same as } \Delta E_{\text{side}} \text{ but for the front and back CV faces}$

$\Delta E_4 = \sum w_i E_i \mu_{\text{en}}(E_i) \frac{e^{-\mu(E_i)L/u_i}}{\mu(E_i)} (1 - e^{-\mu(E_i)s_i})$ of $l = 0$ photons passing
 through the POM circle

$\Delta E_5 = \sum w_i E_i \mu_{\text{en}}(E_i) \frac{e^{-\mu(E_i)L/u_i}}{\mu(E_i)} (1 - e^{-\mu(E_i)h/u_i})$ of $l = 0$ photons passing
 through the POM circle

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$$\Delta E_6 = \sum w_i E_i \mu_{\text{en}}(E_i) \frac{h}{u_i} \text{ of } l = 0 \text{ photons passing through the POM circle.} \quad (4.22)$$

In the above expressions for ΔE_4 , ΔE_5 and ΔE_6 , E_i is the energy of the i 'th photon, $\mu(E_i)$ and $\mu_{\text{en}}(E_i)$ the corresponding attenuation and energy absorption coefficients, u_i the photon direction cosine with respect to the beam axis, w_i its statistical weight, and s_i its path length through the CV. Scoring of these quantities is initiated each time an $l = 0$ photon passes through the POM plane. The distance between the measurement plane and the front face of the CV is denoted with L and the cavity height with h . Note that $\Delta E_2 + \Delta E_{\text{side}}$ is used for the calculation of A_{eloss} and $\Delta E_2 + \Delta E_{\text{side}} + \Delta E_{\text{FB}}$ for A_{cpe} .

Except for the ratios $A_x = A_{\text{att}} \Delta E_g'' / \Delta E_g'$ and $A_{\text{cpe}} = (\Delta E_2 + \Delta E_{\text{side}}) / (\Delta E_2 + \Delta E_{\text{side}} + \Delta E_{\text{FB}})$, the correlation between the various ΔE_j , $j = \text{g, side, FB}, 1 \dots 6$, is strong and/or the ratios defining the various correction factors are close to unity. As a result, a very small statistical uncertainty is obtained quickly for all correction factors except A_x and A_{cpe} . The computation of A_{cpe} is problematic because, although ΔE_{FB} is very small compared to ΔE_2 , it is obtained as

$$\Delta E_{\text{FB}} = \Delta E_{\text{FB,out}} - \Delta E_{\text{FB,in}} . \quad (4.23)$$

The sum of energies of $l = 0$ electrons entering ($\Delta E_{\text{FB,in}}$) and leaving ($\Delta E_{\text{FB,out}}$) the CV is of the same order as ΔE_2 . As a result, the uncertainty of A_{cpe} is of the same order as the uncertainty of ΔE_2 and, so, much larger than the uncertainties of the other correction factors. To improve the efficiency of the computation of A_{cpe} ,

$$\Delta E'_{\text{FB,in}} - \Delta E'_{\text{FB,out}} \equiv 0 \quad (4.24)$$

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is added to the rhs of Eq. (4.23), where $\Delta E'_{\text{FB,in/out}}$ is the energy of $l = 0$ electrons entering/leaving the cavity when photon attenuation is removed. Without photon attenuation there is a perfect balance between these two energies and therefore their difference is manifestly zero as indicated by Eq. (4.24). The front/back face energy imbalance is then computed as

$$\Delta E_{\text{FB}} = \sum_{\text{in}} w_i E_i (\kappa_i - 1) - \sum_{\text{out}} w_i E_i (\kappa_i - 1) \quad (4.25)$$

where the summation is over $l = 0$ electrons with energies E_i , statistical weights w_i and attenuation un-weighting factors κ_i entering (in) or leaving (out) the CV. Because, in practice photon attenuation is not more than a few percent, $\kappa_i - 1 \ll 1$, the uncertainty of ΔE_{FB} is drastically reduced, and the efficiency of the calculation of A_{cpe} is increased by 3 to 4 orders of magnitude.

The computation of the A_x correction factor depends on the technique employed to measure the attenuation correction. The `egs_fac` code offers the ability to calculate A_x for the evacuated-tube technique utilized at NRC. In order to obtain A_x , the user must define three simulation geometries, one for the FAC without the tube present, one with the tube present and filled with air, and one with the tube containing a vacuum. The statistical uncertainty of A_x is dominated by the uncertainties of $\Delta E'_g$ and $\Delta E''_g$ which are only weakly correlated. To improve the efficiency of the A_x calculation, the energies $\Delta E'_g$ and $\Delta E''_g$ in the geometry with the tube filled with air or vacuum are obtained from the corresponding energies $\Delta E'_4$ and $\Delta E''_4$ by applying the appropriate correction factors, *i.e.*,

$$A_x = \frac{\Delta E_5}{\Delta E_6} \frac{\Delta E'_2 + \Delta E'_{\text{side}} + \Delta E'_{\text{FB}}}{\Delta E'_g} \frac{\Delta E''_g}{\Delta E''_2 + \Delta E''_{\text{side}} + \Delta E''_{\text{FB}}} \frac{\Delta E''_4}{\Delta E'_4} \quad (4.26)$$

In the above equation, the convention is used that the quantities with prime and

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double prime have the same meaning as the corresponding quantities without any prime, and that double/single prime is for the situation with the tube filled with vacuum/air. The uncertainty of A_x calculated this way is much smaller. The only slight complication is that, in order to compute the statistical uncertainty of A_x , one needs to compute the covariance matrix for the 8 energies on the rhs of Eq. (4.26), instead of a single covariance term needed for the uncertainties of all other correction factors.

As a final note, the air collision kerma K_{col} is obtained in a separate simulation with the FAC removed using

$$K_{\text{col}} = \frac{1}{\pi R^2} \sum \frac{w_i E_i}{|u_i|} \frac{\mu_{\text{en}}(E_i)}{\rho} . \quad (4.27)$$

4.3 X-ray system simulation

At the medium energies, tube potentials of 120 kV, 150kV, 180kV, 200 kV and 250 kV with an added filtration of 0.4954 mm Cu + 1 mm Al are simulated using the same x-ray system used in Chapter 3, i.e., the COMET MXR-320 x-ray tube. Two reference beam qualities (135 kV and 250 kV), as recommended by the Consultative Committee for Ionizing Radiation¹³³ (CCRI), are also included for comparison with previous EGSnrc calculations of A_{eloss} and A_{scat} by Burns.¹²⁸ Low-energy beam qualities are generated at NRC with a Philips MCN 101 single pole metal-ceramic x-ray tube (100 kV maximum tube voltage). The tungsten anode has an angle of 22° with a focal spot of 1.5 mm by 1.5 mm. The inherent filtration of this x-ray tube is 1 mm of Be. Two sets of beam qualities are simulated in the low-energy range: one set, which will be loosely called “lightly filtered”, with an added Al filtration of 0.2545 mm for tube potentials between 15 kV and 80 kV, and no filtration at 10 kV; and a mammography

set with a 0.0640 mm thick Mo filter and tube potentials between 23 kV and 50 kV.

Rather than using intermediate phase space files as in Chapter 3, BEAMnrc⁹⁵ is used to model the x-ray tubes as a particle source for subsequent simulation of the transport through the FAC¹³⁴ with `egs_fac`. The same MC transport parameters as the ones used in the BEAMnrc simulations of Chapter 3 are used here. The only difference is the use of the `norej` option for Compton scattering which uses the actual cross-sections with binding effects included as explained in section 2.3.5.

The BEAMnrc x-ray tube simulations utilize DBS with a splitting factor NBR SPL of 3×10^5 for the MEES and of 3×10^6 for the LEES calculations. The DBS splitting field radius is set to 13 cm at the medium energies and 5 cm at the low energies. This might appear wasteful considering that the radius of the FAC opening is significantly smaller (see Table 4.1, page 64) and that practically no photons can penetrate the 2 cm thick chamber lead wall beyond the HEVIMET aperture diaphragm (see Table 4.1 for HEVIMET composition). This is shown in Fig. 4.1 for the MEES whose lead wall opening has a radius of 1.25 cm. However, using a smaller DBS splitting field radius increases the chance of “fat” photons interacting in the vicinity of the FAC opening to produce bursts of scattered photons when their interaction is split NBR SPL times. Such bursts, although very rare, compromise the statistics of the computed quantities, thus decreasing the simulation efficiency. To avoid following too many photons hitting the chamber geometry outside of the HEVIMET diaphragm, the cutout option of the BEAMnrc simulation source provided by the EGSnrc C++ class library⁷⁶ is employed and the cutout is set to a square with size of 3 cm completely covering the HEVIMET diaphragm.

In Chapter 3, range rejection was used in the BEAMnrc simulation of the x-ray tubes for all electron energies under the assumption that it had a negligible effect on the air-kerma or the particle fluence and that it increased the efficiency significantly.

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Figure 4.1: Photon fluence as a function of position behind MEES lead front wall. Most photons go through the 0.5 cm radius aperture opening. Calculations done with cavity using BEAMnrc as a source for a Comet MXR-320 x-ray tube at 250 kV. The fluence profile was extracted from a phase space file using the utility code `beamdp`.

This assumption was based on calculations using DBS with a very conservative splitting number of 10^4 for these beam energies and statistical uncertainties of about 2%. These calculations showed efficiency increases of 2 to 5 times when using range rejection for 50 kV and 200 kV beams respectively. More accurate calculations for 20 kV and 200 kV, using DBS parameters closer to the optimum values for maximum efficiency, reveal that there is a non-negligible 0.65% effect on the FAC dose and the air-kerma at the POM for the 200 kV beam and no effect at 20 kV within the one sigma uncertainty of 0.06%. The efficiency improvement is not as dramatic as before, being 25% at 20 kV and 85% at 200 kV. For this reason, an ESAVE of 0.531 MeV is used at the medium energies since no photon with less than 10 keV reaches the POM and no range rejection is used at the low energies.

4.3. X-RAY SYSTEM SIMULATION

4.4 FAC chamber modeling

The Canadian standards for low and medium x-ray beam qualities, the LEES and the MEES FACs respectively, are in-house developments at the NRC, where they are still maintained. A schematic representation of the MEES is shown in the upper panel of Fig. 4.2 with its main dimensions. More details can be found in the paper by B. Henry and C. Garret.¹³⁵ The LEES is almost identical in design to the MEES, but much smaller. Table 4.1 provides the most important dimensions of the LEES and the MEES.

Table 4.1: Main characteristics of the LEES and MEES Free Air ionization Chambers. Diaphragms made out of HEVIMET, a tungsten carbide alloy whose chemical composition is taken in this work as 90% tungsten, 5% nickel and 5% copper. HEVIMET is machinable and is usually sintered from powdered tungsten and powdered copper, it is a biologically safe, very heavy material.

Parameter	LEES	MEES
Collector length (cm)	4.60	10.20
Aperture diameter (cm)	0.50	1.00
Air attenuation length (cm)	9.90	41.90
Plate separation (cm)	6.10	35.00
Diaphragm inner radius (cm)	0.25	0.50
Diaphragm outer radius (cm)	2.37	2.00
Diaphragm thickness (cm)	0.64	1.25
Lead wall opening (cm)	2.00	1.25

These FACs are modeled with the geometry module of the C++ EGSnrc

library, `egspp`.⁵⁷ A view of the chamber model employed in this investigation for the MEES is shown in the lower panel of Fig. 4.2. The simulation of the radiation transport through the FAC geometry with the `egs_fac` user-code utilizes the photon splitting technique from section 2.2.1 to improve the efficiency of the dose estimation in the collecting volume. In addition, `rr+RR` is applied to electrons that are farther away from the CV than their CSDA range as discussed in section 2.2.4. All EGSnrc transport parameters are set to their default values except that Rayleigh scattering, which is not included by default, is turned on, and Compton binding effects are taken into account using the `norej` option instead of the default option `on`. Particle production and transport threshold energies are 1 keV kinetic energy for photons and electrons.

The medium energy range is initially selected because measured corrections are believed to be accurate. A good agreement with measurements will therefore establish the validity of the approach and the correctness of its implementation. At these beam qualities, all correction factors are computed to a negligible statistical uncertainty, except for one sigma uncertainties of $\sim 0.005\%$ (A_{scat}) and $\sim 0.006\%$ (A_x). To achieve this statistical precision, of the order of 1×10^9 photons incident on the FAC are required, and the simulation takes about 15 hours per beam quality on a cluster with 80 Intel Xeon 5460 calculation cores (3.16GHz). Without the computation of A_x the simulation time is reduced by a factor of 3.

Once the proposed methodology is validated in the medium energy range, it is used to determine a consistent set of MC calculated correction factors for the LEES irradiated by the two different sets of low-energy beam qualities, produced with the Philips x-ray tube MCN 101. At these lower energies, some of the corrections which are unity in the medium energy range, can potentially become non-negligible.

All FAC correction factors are computed to better than a one sigma uncer-

4.4. FAC CHAMBER MODELING

Figure 4.2: Upper panel: Schematic horizontal sectional view of the MEES used at NRC. Taken from the paper by B. Henry and C. Garret.¹³⁵ Lower panel: Sectional view of the geometrical model of the MEES visualized using `egs.view`, the `egs++` geometry viewer.

4.4. FAC CHAMBER MODELING

tainty of $\sim 0.005\%$ with exception of A_x and A_b for which the one sigma uncertainty is better than $\sim 0.01\%$. To achieve this statistical precision, between 4×10^9 and 8×10^9 photons incident on the FAC are required, and the simulation takes between 5 and 15 hours per beam quality on a cluster with 264 Intel Xeon 5460 calculation cores (3.16GHz).

The initial A_b values were obtained using two separate calculations as described in section 4.2. One calculation was done with `egs_fac` for the collision air kerma with the FAC present and another with `cavity` to determine the air collision kerma when no FAC is present. Calculating A_b this way requires a huge effort since one cannot take advantage of possible correlations. For instance, to achieve a statistical precision of 0.024% , for the 23 kV mammography beam, 8×10^9 photons incident on the FAC are required and the simulation takes about 52 hours for the two separate calculations on a cluster with 264 Intel Xeon 5460 cores (3.16GHz). To improve the efficiency of this calculation, `egs_fac` was modified to allow calculating the collision air kerma at the POM including scattered photons. This way one can perform both calculations with the same user-code and take advantage of the correlations. For the beam quality mentioned above, an uncertainty of 0.0074% for A_b can be obtained with 8×10^9 incident photons in almost half the time as before thus showing an efficiency increase of about 20 times.

4.5 MEES correction factors

Using the methodology described in the previous sections, FAC correction factors are calculated for the NRC MEES irradiated with a Comet MXR-320 x-ray tube. The correction factor for backscattering, A_b , is found to be unity for the 120 kV and 250 kV beam qualities. The correction factor for geometrical effects, A_g , is negligible (2

parts in 10^5 or less) for all investigated beam qualities. Note, however, that this study ignores off-focal radiation from the x-ray tube produced by backscattered electrons re-entering the target and/or target supporting structure due to the presence of the accelerating electric field. Simulations taking into account the off-focal radiation are therefore needed before dismissing the need to take into account A_g .

Figure 4.3: The CPE correction A_{cpe} as a function of tube potential. Note that $(A_{\text{cpe}} - 1) \times 10^4$, not A_{cpe} itself, is shown. One sigma statistical uncertainties are less than 0.001%.

Figure 4.3 shows the calculated A_{cpe} , which corrects for the lack of charged particle equilibrium along the beam axis. This correction is very small in the entire energy range considered, only departing from unity by 1.5 parts in 10^4 at 250 kV. In Ref.,¹²⁷ an analytic expression for A_{cpe} was derived for a very simple model. In this

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model, A_{cpe} is given by

$$A_{\text{cpe}} = \frac{e^{\mu R} - 1}{\mu R} \approx 1 + \frac{\mu R}{2} + \frac{\mu^2 R^2}{6} + \dots \quad (4.28)$$

with μ being the linear attenuation coefficient and R the electron CSDA range. Eq. (4.28) gives an indication of the energy dependence of A_{cpe} . In a more realistic scenario, the electron range R has to be replaced with the average penetration depth d in air of electrons set in motion by the incident beam in Eq. (4.28). The product μd increases with increasing photon energy, except for photon energies below ~ 5 keV, where the strong increase of μ with decreasing energy outweighs the decrease in d . Thus, the CPE correction may become not completely negligible for higher kV or more heavily filtered beams.

Calculations performed without the electrodes or without the guard bars for a 250 kV beam quality show no difference to the simulations with full details included. This suggests that the much simpler FAC models employed in previous investigations are adequate. On the other hand, the difference in simulation time between a simple and a complex FAC model is only a few percent, so one can also use the full model without significant loss in simulation efficiency.

4.5.1 Correction factors used for the primary standard

From the corrections proposed in this work, only A_{att} , A_{scat} and A_{eloss} are currently used in the NRC primary standard. While A_{att} has been recently determined experimentally at our lab, A_{scat} and A_{eloss} are derived from the data by Wyckoff and Attix.¹²¹ These authors provide a limited set of experimental data for different beam qualities. At our lab these data have been fitted to analytical expressions and used to derive these corrections for an arbitrary beam quality. Systematic uncertainties of

Figure 4.4: Comparison of MC calculated values of the MEES FAC correction factors for an MXR-320 Comet x-ray tube with the values currently in use at our lab for routine calibration. Open symbols are the MC calculations and solid symbols the experimental values. The combined uncertainty of the total measured correction is 0.17% and is shown by error bars. The statistical uncertainties of the computed values are less than 0.005%.

0.2% and 0.1% are assigned to A_{scat} and A_{eloss} respectively.

Figure 4.4 compares these experimental correction factors to those obtained from the MC simulations. An excellent agreement within the statistical and experimental uncertainties is observed for all three correction factors and also for their combined effect, which ranges from a 0.06% overestimation at 120 kV to a 0.08% underestimation at 250 kV. The level of agreement observed contrasts with the estimate of the experimental uncertainties which seems conservative.

The attenuation correction is the largest correction followed closely by the

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scatter correction, although they affect the chamber reading in opposite ways, effectively reducing their total effect. A_{eloss} is the smallest correction factor of these three, ranging from unity at 120 kV up to 0.9983 at 250 kV (a 0.17% correction). The slow variation of these corrections in a relatively large range of x-ray tube potentials is due to the fact that the average energy of these beams lies in a much narrower interval from around 68 keV up to 100 keV.

Correction factors for two CCRI reference beam qualities (135kV and 250 kV) calculated for the MEES are compared in table 4.2 with the values calculated by Burns¹²⁸ for A_{eloss} and A_{scat} using EGSnrc. To obtain A_{scat} from Burns' values one must use the inverse of their $k_{\text{scat}} \cdot k_{\text{flu}}$ values. Note that Burns quotes total uncertainties, whereas our uncertainties are only statistical. The excellent agreement between Burns' and our values confirms that the simple chamber model used by Burns has a negligible effect on the calculated corrections.

Table 4.2: Comparison of current calculations of scatter and electron loss corrections for two CCRI beam qualities with the values obtained by Burns.¹²⁸ Note that Burns' scatter correction has been multiplied by the correction for photon fluorescence. While Burns quotes total uncertainties, our uncertainties are only statistical (one sigma).

tube potential (kV)	A_{eloss}		A_{scat}	
	Burns	this study	Burns	this study
135	0.9999[5]	0.99993[0]	1.0072[5]	1.00723[6]
250	0.9973[5]	0.99750[3]	1.0043[5]	1.00455[6]

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4.5.2 Inconsistency of evacuated-tube technique at medium energies

Considering that the use of a computed instead of a measured A_{att} , or the alternative introduction of the A_x correction factor, is the most significant departure from previous work proposed here, a more detailed consideration of the attenuation correction factor is in order. Figure 4.5 shows a comparison between the measured and computed attenuation correction.

Figure 4.5: Comparison between measured (filled triangles) and calculated (circles) attenuation correction factors for the MEES. The filled circles correspond to A_{att} computed directly as the ratio $\Delta E_5/\Delta E_6$ from Eq. (4.11) and (4.13), the open circles are from the ratio $\Delta E'_g/\Delta E''_g$, which corresponds to the experimental procedure.

Unlike Fig. 4.4, where the overall uncertainty assigned to the experimental

determination of A_{att} is shown, in this figure the error bars on the experimental data ($\sim 0.01\%$) depicted with filled triangles corresponds to the precision with which the ratio of ionizations in the two irradiations (brass tube filled with air or vacuum) can be measured. The attenuation correction computed directly in the simulation as the ratio $\Delta E_5/\Delta E_6$, with ΔE_5 and ΔE_6 defined in Eq. (4.11) and (4.13), is systematically lower by between 0.03% and 0.04% compared to the measurements. However, when the experimental procedure used to determine A_{att} is simulated, the computed $\Delta E'_g/\Delta E''_g$ ratio matches the experiment within 0.01% or better, except for 150 kV where the difference is about 0.02% . The difference between the filled and open circles is the A_x correction discussed in section 4.1. Within the statistical uncertainty of 0.006% , the computed A_x can be considered to be 0.9997 for all investigated beam qualities.

4.5.3 Correction factor for aperture leakage A_{ap}

Calculated values for the aperture correction A_{ap} are shown in figure 4.6. Even at the lowest tube potential, A_{ap} is already 1.00055 and for the highest tube potential it becomes more than twice as large ($A_{\text{ap}} = 1.0013$). Therefore, including A_{ap} in the overall correction will have a non-negligible impact, shifting the total correction closer to unity.

The goal of a FAC design is to have a thick enough front wall in order to reduce the amount of stray radiation to a negligible amount, only allowing photons getting through the aperture to reach the collecting volume. However, as previously reported by Grimbergen *et al.*,¹²⁴ some photons leak through the HEVIMET body of the diaphragm not backed by the lead wall (see Fig. 4.1 on page 63). To estimate the maximum contribution from this leakage, A_{ap} is calculated for the hardest beam in this study (250 kV) for different field sizes. When the beam is restricted to just

Figure 4.6: Calculated aperture correction A_{ap} for the MEES irradiated by different x-ray beam qualities. One sigma statistical uncertainties are equal or less than 0.0007%

the diaphragm opening, the aperture correction is about 0.08%. This correction only accounts for photons bouncing off the opening surface of the diaphragm, or entering the diaphragm opening at an angle oblique to its surface. For field sizes covering the whole opening of the lead box (1.25 cm radius) the contribution from stray radiation is about 0.05%. A similar finding was obtained by Grimbergen *et al.*, who found that the transmission through the rim of the diaphragm is the major process up to 250 keV. Kurosawa and Takata¹³⁰ published a MC study (based on MCNP4B¹³⁶) of the corrections needed to account for stray radiation and photon scatter off the diaphragm opening surface for the medium- and low-energy FACs in use at the National Metrology Institute of Japan (NMIJ). Table 4.3 shows a comparison of our aperture corrections for the MEES for two CCRI beam qualities (135 kV and 250 kV) with the values obtained by these authors for the medium-energy FAC used

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at NMIJ. Their values are consistently larger than ours. This increased contribution from the aperture can be partially explained by the thicker diaphragm of the NMIJ chamber (20 mm *vs* 12.5 mm). However, one would expect less stray radiation from the NMIJ chamber, which accounts for 0.07% of the aperture correction at 250 kV for this chamber,¹³⁰ in contrast with a 0.05% contribution for our chamber.

Table 4.3: Comparison of current calculations of aperture corrections for two CCRI beam qualities with the values obtained by Kurosawa and Takata¹³⁰ for a medium-energy FAC used at NMIJ with the same diameter aperture as the MEES. No uncertainties are quoted by these authors. Our uncertainties are only statistical (one sigma).

tube potential (kV)	A_{ap}	
	Kurosawa and Takata	this study
135	1.0013	1.00051[1]
250	1.0025	1.00163[2]

4.5.4 Self-consistency of EGSnrc electron transport algorithm

Before concluding this section, a remark on the efficiency enhancing methods employed to calculate A_{cpe} and A_{x} discussed in section 4.2 is in order. These methods rely upon the energy depositions $\Delta E_2 + \Delta E_{\text{side}} + \Delta E_{\text{FB}}$, computed including electron transport, and ΔE_4 , calculated with photon transport only, to be equal. This condition will only be satisfied if the condensed history simulation of electron transport is completely self-consistent and artifact-free. This issue has been discussed extensively in previous publications,^{22,131} where the self-consistency of the EGSnrc electron transport methods were demonstrated at the 0.1% level. Given the much higher computing power available today, the self-consistency check can be undertaken to a much lower

statistical uncertainty compared to the initial EGSnrc publications. Very long simulations for the highest and lowest energies considered in this investigation were run and the consistency between $\Delta E_2 + \Delta E_{\text{side}} + \Delta E_{\text{FB}}$ and ΔE_4 verified to be satisfied within a statistical precision of 0.005%.

4.6 LEES correction factors

Two significantly different sets of low-energy beam qualities are used in these calculations. This can be seen in Fig. 4.7 where the 50 kV spectra for two beam qualities with 0.2545 mm Al and 0.064 mm Mo added filtration are shown. The molybdenum K absorption edge filters out a significant fraction of the x-rays with energies near 20 keV, the K edge energy of Mo. At around 17.4 keV the combined contribution from the Mo K-lines can be observed since the 0.25 keV resolution used to score the spectra is not enough to separate the K_α (17.479 keV) and K_β (17.374 keV) lines. Characteristic L lines for tungsten can be clearly seen in the lower end of the softer Al filtered spectrum. The HVL in terms of mm of Al is 0.527 mm for the Mo filtered beam ($E_{\text{eff}} = 17.7$ keV), and 0.337 mm for the Al filtered beam ($E_{\text{eff}} = 15.1$ keV).

The corrections for lack of CPE, A_{cpe} , and for geometrical effects, A_{g} , are negligible for both sets of beam qualities. A_{cpe} is less than 7 parts in 10^5 for all beam qualities and A_{g} is less than 8 parts in 10^5 for the mammography beam qualities and less than 1.5 parts in 10^4 for the lightly filtered beams. These corrections have been calculated to a statistical uncertainty better than 0.0003%.

Figure 4.7: 50 kV x-ray spectra at 1 m from a Philips MCN 101 x-ray tube for two beam qualities with added filtration of 0.2545 mm of Al and 0.064 mm of Mo respectively.

4.6.1 Correction for attenuation A_{att}

4.6.1.1 Tube length correction

The tube used in the evacuated-tube technique for determining A_{att} is not the same length as the distance from the POM to the center of the sensitive volume L . While L is 9.9 cm, the actual length of the tube l is 11.1 cm. Under “narrow-beam attenuation” conditions, $A_{\text{att,exp}}$ can be assumed to follow an exponential attenuation law and therefore the following identity should be valid

$$\frac{\ln A_{\text{att,exp}}^L}{\ln A_{\text{att,exp}}^l} \cdot \frac{l}{L} = C, \quad (4.29)$$

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Figure 4.8: **Circles (y-axis on left):**Evaluation of Eq. (4.29) for the lightly filtered low-energy beams for tubes of length $l = 11.1$ cm and $L = 9.9$ cm. One sigma statistical uncertainties are better than 0.4% **Squares (y-axis on right, same scale):** Effect of assuming C unity on $A_{att,exp}$.

with $A_{att,exp}^L$ and $A_{att,exp}^l$ the attenuation corrections obtained with the evacuated-tube technique for tubes of length L and l respectively. C should approach unity the better the experimental setup fulfills the requirements for “narrow beam attenuation”. The current NRC $A_{att,exp}$ values were obtained from measured values for a tube of length l corrected using Eq. (4.29) assuming C unity.

To test the validity of this assumption MC calculated $A_{att,exp}$ values for tubes of length L and l were used to evaluate Eq. (4.29). This is shown in Fig. 4.8 with circles for the lightly filtered beams. The experimental setup employed in the evacuated-tube technique deviates about 1% from ideal “narrow-beam attenuation”. $A_{att,exp}$ values were derived from the ratio of direct MC A_{att} to A_x values. The uncertainty in A_{att} is less than 0.002% and in A_x less than 0.008%. However, this still results in

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an uncertainty for C of about 0.4%.

From Eq. (4.29) follows that the effect on $A_{att,exp}^L$ of assuming C to be unity, ζ can be obtained as

$$\zeta = (A_{att,exp}^L)^{\frac{1}{L} \cdot (C-1)} - 1, \quad (4.30)$$

and is shown to be less than 0.05% in Fig. 4.8 (squares) for the lightly filtered x-ray beams.

4.6.1.2 Lightly filtered beam qualities

Attenuation corrections obtained from experimental measurements at our lab in the 1990s for the low-energy lightly filtered beam qualities are compared with MC calculated values in Fig. 4.9. At 20 kV and higher tube potentials, the direct MC calculations (solid circles) predict systematically higher A_{att} values than the measurements (triangles). These differences increase with tube potential from 0.07% at 20 kV to a maximum overestimation of 0.32% at 70 kV. Below 20 kV, the MC values underestimate measured A_{att} values by as much as 1.76% at 10 kV. Accounting for the inconsistency introduced by the evacuated-tube technique increases the MC calculated values (open circles) and as a consequence these values lie even further apart from the experimental values above 20 kV increasing the maximum difference to 0.45% at 70 kV. The underestimation observed at 10 kV and 15 kV is reduced to 0.64% and 0.16% respectively. To put such discrepancies into perspective, one should note that a 0.45% difference in A_{att} at 70 kV translates into a 15.5% difference in the actual attenuation, and a 0.64% difference in A_{att} at 10 kV translates into a 4.5% difference. The observed differences suggest the simulations predict harder spectra over 20 kV, and softer spectra below. This behavior cannot be explained by a wrong filter or absorber thickness since in that case all simulated spectra would be either harder or softer.

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Figure 4.9: Comparison between measured (filled triangles) and calculated (circles) attenuation correction factors for the LEES. The filled circles correspond to A_{att} computed directly as the ratio $\Delta E_5/\Delta E_6$ from Eq. (4.11) and (4.13), the open circles are from the ratio $\Delta E'_g/\Delta E''_g$, which corresponds to the experimental procedure.

Photon cross section uncertainties: These discrepancies are significant for the accuracy level required at a standards lab and cannot be solely explained by the uncertainties in the photon cross sections which are expected to be larger at lower energies. A rough estimate of the envelope of uncertainty for the photo-electric cross sections provided in the EPDL photon data library has been reported by Cullen *et al.*¹³⁷ These authors quote a 5% uncertainty in the energy range from 1 keV to 5 keV and a 2% uncertainty in the 5 keV to 100 keV energy range. These uncertainty estimates also apply to the XCOM compilation of photon cross sections used in our calculations because its photo-electric cross sections are derived from the same sources as the EPDL compilation. Since the photo-electric effect is the dominant interaction

at these low energies, where the uncertainties are the largest, Hubbell¹³⁸ proposes to use this uncertainty estimate as a very rough subjective guide to the uncertainty in the total photons cross sections.

Under "narrow beam attenuation" conditions, $A_{\text{att,exp}}$ will follow an exponential attenuation law with an equivalent attenuation coefficient μ_{eq} , i.e.,

$$A_{\text{att,exp}} = e^{-\mu_{eq}L} . \quad (4.31)$$

Under this assumption, a 1% uncertainty in the attenuation coefficient will affect $A_{\text{att,exp}}$ at 80 kV by only 0.03% and by 0.15% in the extreme assumption of a 5% uncertainty in the whole energy range. Based on Eq. (4.31), to account for the 0.45% discrepancy observed at 70 kV, the attenuation coefficient would have to be wrong by 15%.

If the x-ray spectrum at the POM $\phi(E, POM)$ and the relative cross section uncertainty ε_i at energy E_i were known, one could analytically estimate the impact of these uncertainties on $A_{\text{att,exp}}$ using

$$A_{\text{att,exp}} = \frac{\sum_i \left(\frac{\mu_{en}}{\rho} \right)_i \cdot E_i \cdot \phi(E_i, POM) \cdot e^{-\mu_i(1 \pm \varepsilon_i)L} \cdot \Delta E_i}{\sum_i \left(\frac{\mu_{en}}{\rho} \right)_i \cdot E_i \cdot \phi(E_i, POM) \cdot \Delta E_i} , \quad (4.32)$$

where μ_i is the linear attenuation coefficient of air for energy E_i , $\phi(E_i, POM)$ the photon fluence for this energy at the POM, and $\left(\frac{\mu_{en}}{\rho} \right)_i$ the corresponding mass energy absorption coefficient. For the 10 kV spectrum, all the terms in the numerator will fall in an energy region where the uncertainties and the attenuation coefficient are the largest. For increasing tube potential more terms in the numerator will lie in the energy region with smaller uncertainty and decreasing attenuation. Hence, one would

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expect to see smaller discrepancies with the experiment for increasing tube potential.

Tungsten/rhenium target: The x-ray tube anode is constructed of high temperature materials. The focal spot temperature can reach 2500 °C during an exposure, and the anode assembly can reach 1000°C following a series of large exposures. Typically, anode materials are a mixture of 90% tungsten with 10% rhenium. The rhenium makes the tungsten more ductile and resistant to wear from the impact of the electron beams. A MC $A_{\text{att,exp}}$ calculation for such a target composition at 80 kV tube potential was compared with the value for a pure tungsten target showing no effect at the one sigma 0.007% level.

Contamination of exit window with tungsten: The continuous operation of an x-ray tube causes tungsten to be deposited from the target onto the interior surface of the tube. The thin tungsten layer will slowly darken the tube and has been thought to degrade the quality of the x-ray beam. However, this tungsten buildup on the exit window would harden rather than soften the x-ray beam. Stears *et al.*¹³⁹ studied the effect of tungsten deposited on the x-ray tube windows by analyzing radiographs and HVL measurements along with the HVL data from approximately 200 functioning x-ray tubes used in many applications that were monitored for more than 8 years. These researchers did not find a significant increase in HVL with diagnostic x-ray tube use.

Sensitivity to BEAMnrc \$BDY_TOL parameter: An artificial beam hardening could also be caused by the boundary tolerance parameter \$BDY_TOL used in BEAMnrc when simulating the x-ray tube. This parameter defines the distance a particle is pushed inside a geometrical region to avoid round-off errors when crossing boundaries. Its default value is set to 10^{-5} cm and may be too large in the energy

Figure 4.10: Comparison of two direct A_{att} MC calculations using different $\$BDY_TOL$ values in BEAMnrc. Negligible statistical uncertainties are masked by the symbols and not visible.

range considered in this work. If electrons are pushed too far inside the tungsten target, the bremsstrahlung photons will travel more inside the target. To check the impact of this parameter, direct A_{att} calculations with $\$BDY_TOL = 10^{-6}$ cm for 20 kV, 50 kV and 80 kV are compared with the initial calculations. As can be seen in Fig. 4.10 there is no effect in A_{att} when reducing $\$BDY_TOL$ by a factor of 10.

Sensitivity of A_{att} to EII: The total EII cross section in the kilovoltage energy range increases with electron energy as shown in Fig. 2.3 (page 25) for copper and gold. The direct impact of this type of interaction on the bremsstrahlung spectrum is the appearance of characteristic x-ray lines from the different atomic shells. This can be seen in the tungsten x-ray spectra of Fig. 4.11 for 10 kV, 50 kV and 80 kV, calculated with the C++ user-code `cavity` using BEAMnrc as a particle source.

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Figure 4.11: MC calculated tungsten x-ray spectra for a Philips MCN 101 x-ray system at 10 kV tube potential without Al filtration, and at 50 kV and 80 kV tube potentials with a 0.2545 mm Al filtration. Spectra obtained with user-code `cavity` using BEAMnrc as a particle source. Fluence for the 10 kV beam has been multiplied by a factor of 10 for visibility.

Tungsten K-shell and L-shell characteristic x-rays can be seen for the 80 kV spectrum. Spectra generated with tube potentials below 60 kV will not display the K-shell lines since not enough energy will be available for these transitions. One can thence assume that EII could potentially affect A_{att} differently at different energies.

To test this assumption, $A_{\text{att,exp}}$ calculations were done without inclusion of the EII interaction and compared with the initial simulations. Fig. 4.12 shows the effect on $A_{\text{att,exp}}$ of turning off EII. The attenuation correction factor is larger than when including EII, pointing to a hardening of the x-ray beams. The increase of $A_{\text{att,exp}}$ is only 0.052% at 10 kV well within the one sigma uncertainty of 0.055% at

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Figure 4.12: Effect of EII on MC calculated LEES $A_{\text{att,exp}}$ corrections for the lightly filtered x-ray beams.

this energy for the calculations without EII. This increase goes from 0.2% at 15 kV up to 0.6% at 80 kV.

The hardening of the spectra and the energy dependent effect of EII on $A_{\text{att,exp}}$ support the idea that an increase of the tungsten L-shell EII cross-sections would have the opposite effect to turning off EII, bringing it closer to the experimental values. That only the tungsten L-shell EII cross-sections needs to be increased can be inferred from two facts. Firstly, no tungsten K-lines are observed below 60 kV and hence, no effect on $A_{\text{att,exp}}$ would be seen below this tube potential by modifying the tungsten K-shell EII cross sections. Secondly, the hardening effect is observed in the entire energy range when EII is turned off. Calculations for varying scaling factors of the tungsten K-shell EII cross section at 80 kV showed no effect on $A_{\text{att,exp}}$. Scaling the

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tungsten L-shell EII cross-sections will not affect the results from section 4.5 for the medium energy beams since the 0.4954 mm Cu filters out all photons below 20 keV.

Optimum L-shell EII cross section scaling factor: EGSnrc reads in the relative EII cross sections for the K , L_I , L_{II} and L_{III} shells. These cross sections are normalized to the maximum cross section, which is also read from the EII cross section file. Therefore, one way to modify any of the EII cross sections is to multiply the corresponding maximum EII cross section by a scaling factor f_{EII} .

To find the optimum scaling factor, MC calculated values of $K_{att,exp}$ using different scaling factors were compared with the measured value for the 80 kV, 70 kV and 20 kV beam qualities ($K_{att,exp}$ is just the inverse of $A_{att,exp}$). The ratio of the calculations to the measurements is shown in Fig. 4.13. The data for 80 kV

Figure 4.13: Relative difference of MC calculated $K_{att,exp}$ with measured values for different values of the tungsten L-shell EII scaling factor f_{EII} at 80 kV, 70 kV and 20 kV.

and 70 kV indicate that a scaling factor of 1.8 produces the best agreement with the measurement. However, in the case of the 20 kV beam, a larger scaling of 1.9 seems to work best, although the statistical uncertainties are still significant. One can also hypothesize that at lower energies, where EII becomes less relevant, the larger uncertainty in the photon cross sections becomes the more dominant source of uncertainty.

Calculations of $A_{\text{att,exp}}$ for several scaling factors are graphically compared to the measured values in Fig. 4.14, confirming that a value of 1.8 brings the calculations in close agreement with the experimental values especially at the higher tube potentials. At low tube potentials the sensitivity to changes in the scaling factor f_{EII} is less, especially at 10 kV where almost no change in $A_{\text{att,exp}}$ is seen.

Plotting the relative differences with the experimental data as shown in Fig. 4.15 offers a quantitative overview of the level of agreement between calculations and experiment. The agreement with the experiment for $f_{\text{EII}} = 1.8$ is better than 0.05% (one sigma uncertainty) over 20 kV and about 0.15% for $f_{\text{EII}} = 2.1$. A marked underestimation remains for the 15 kV and 10 kV beam qualities.

There is a clear insensitivity at 10 kV to changes in the tungsten L-shell EII cross-sections suggesting the 0.5% discrepancy with the experiment could potentially be caused by the larger uncertainties in the photon cross sections at low energies. Moreover, any possible effect of increasing the tungsten L-shell EII cross-sections would affect $A_{\text{att,exp}}$ at 10 kV in exactly the opposite way as it would at the other energies. A close look at the spectrum for the 10 kV beam in Fig. 4.11 (page 84) reveals that the L-shell lines would lie on the high energy end of the 10 kV spectrum and thus any potential effect of increasing the tungsten L-shell EII cross-sections would be to harden the spectrum and therefore increase $A_{\text{att,exp}}$.

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Figure 4.14: Comparison of MC calculated $A_{att,exp}$ values with measured values for different tungsten L-shell EII scaling factors f_{EII} . Statistical uncertainties are smaller than symbols and therefore not visible.

4.6.1.3 Mammography beam qualities

LEES attenuation correction measurements for seven mammography beam qualities were performed recently at the NRC. To this end, high purity molybdenum was purchased and precisely machined to a square absorber. The thickness of this absorber was accurately determined by direct caliper measurements and by weighing the absorber. Both methods agree within a tenth of a percent.

Experimental A_{att} values are compared in Fig. 4.16 with MC calculations using default EGSnrc EII cross sections. At these beam qualities, the attenuation correction needed is not as large as for the softer lightly filtered beams. The directly calculated A_{att} values are in closer agreement with the measurements than the A_{att}

Figure 4.15: Percentage difference of MC calculated $A_{att,exp}$ values with measured values for tungsten L-shell EII scaling factors f_{EII} of 1.8 and 2.1.

values calculated modeling the evacuated-tube technique. These latter values overestimate the measurements by about 0.07% except at 23 kV where the overestimation is 0.12%. Discrepancies at these beam qualities are significantly smaller than for the beams in the previous section which is consistent with the small contribution of the L-shell lines to the spectrum as shown in Fig. 4.7 on page 77. It should also be noted that the differences observed for these beam qualities are within the two sigma experimental uncertainties. The A_{att} experimental data in Fig. 4.16 show a deeper drop at 23 kV, which could be due to the uncertainties, but it could also be connected with the proximity of the maximum spectrum energy to the Mo K-shell (see Fig. 4.17). The calculations predict less of a drop and a harder spectrum, i.e., less attenuation. Hubbell¹³⁸ suggested the 2-5% envelope of uncertainty in the photon cross

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Figure 4.16: Comparison between measured (triangles) and calculated (circles) LEES attenuation correction factors for the mammography beams. The open circles correspond to A_{att} computed directly as the ratio $\Delta E_5/\Delta E_6$ from Eq. (4.11) and (4.13), the solid circles are from the ratio $\Delta E'_g/\Delta E''_g$, which corresponds to the experimental procedure. Default EGSnrc EII cross sections were used in this calculations.

sections estimated by Cullen *et al.*¹³⁷ for the photo-electric effect must have ignored uncertainties just above the absorption edges where the uncertainties are significantly larger. A reason for this larger discrepancy at 23 kV could be caused by the simulations allowing too many photons through the Mo filter because the photo-electric cross section near the Mo K-shell may be too small.

Making use of the results from the previous sections, direct A_{att} values were obtained for different f_{EII} values. As the graph in Fig. 4.18 shows, scaling the tungsten L-shell EII cross-sections has not as large an effect on A_{att} as for the lightly filtered beams. Increasing the tungsten L-shell EII cross-sections by a factor of 2.6 causes a

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Figure 4.17: MC calculated tungsten x-ray spectra for Philips MCN 101 at 23 kV tube potential and 0.064 mm Mo filtration. User-code `cavity` and `BEAMnrc` were used in the simulations.

maximum decrease in A_{att} at 50 kV of 0.065% and of only 0.026% at 23 kV. Given that the sensitivity of A_{att} to changes in f_{EII} is within the statistical uncertainties of the experimental data, it is not clear which value reproduces the measurements the best. To be consistent with the results for the lightly filtered beams, a scaling factor f_{EII} of 1.8 is chosen, as there is no evidence from these data indicating the scaling factor should vary with beam quality. A_{att} values calculated using this scaling factor are shown in Fig. 4.19 together with the experimental results for comparison.

4.6.2 Inconsistency of the evacuated-tube technique at low energies

As shown in previous sections, there is an inconsistency in the way the attenuation correction is determined experimentally by accounting for the beam attenuation be-

Figure 4.18: Effect of changing f_{EII} on A_{att} for the mammography beam qualities. Only values for a direct calculation of A_{att} are shown.

tween the POM and the center of the FAC's sensitive volume. This inconsistency is very small in the medium-energy range and the mammography low-energy beams. However, for softer beams this inconsistency cannot be neglected anymore as evidenced by Fig. 4.20 which compares A_x^{-1} values for all these beam qualities. The correction needed due to this inconsistency for the lightly filtered beams is about 0.2% except for the 10 kV beam. At this beam quality, this correction becomes as large as 1.0%.

This implies that, at a primary standards lab where the evacuated-tube technique is used for A_{att} determination, care must be taken to ensure that A_x is included among the FAC corrections in the low-energy range, especially for soft beams. The increasing trend of this correction towards softer beam qualities confirms the sim-

Figure 4.19: Comparison of MC calculated A_{att} values for the mammography beam qualities using $f_{EII} = 1.8$ with the experimental values.

ple model in Ref.,¹²⁷ which predicts that the inconsistency of the evacuated-tube technique is proportional to the linear attenuation coefficient μ .

In this section, the results for the corrections in use at our lab, A_{scat} and A_{eloss} , are discussed and compared with experimentally derived values. These values were derived from the work by Ritz¹²³ in 1959 who provided experimental data for beam qualities from 20 kV up to 100kV with a filtration of 2 mm Be up to 2 mm Be + 4 mm Al. At our lab these data have been fitted to analytical expressions using the commercial software TableCurve 2D[®] by Systat Software Inc.(SSI) and used to derive these corrections for an arbitrary beam quality. For this reason, systematic uncertainties of 0.2% and 0.1% are assigned to A_{scat} and A_{eloss} respectively.

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Figure 4.20: Inverse of MC estimated inconsistency A_x in the experimental determination of A_{att} . Values shown for the medium- and low-energy range beam qualities investigated in this work.

4.6.2.1 Lightly filtered beam qualities

Figure 4.21 shows a comparison of MC calculated correction factors for scatter A_{scat} and electron loss A_{eloss} with values currently in use at our lab. The MC calculated A_{scat} values overestimate the experiment derived systematically by about 0.1%, although they still lie within the stated one sigma uncertainty of 0.2% for the experimental values. Except for beam qualities below 20 kV, where the interpolation is not valid anymore given the limitation in the data provided by Ritz. The one sigma uncertainties in the MC calculated values are less than 0.02%.

4.6.3 Correction for scatter A_{scat} and electron-loss A_{eloss}

The correction factor for electron loss is unity up to the 50 kV beam showing that the plate separation of the LEES is adequate for these beams. However, for higher energy beams this correction becomes non-negligible. For instance, for the 80 kV beam the MC calculations estimate a 0.22% correction and the measurement derived value a 0.12% correction. Values derived from the experiment have assigned one sigma statistical uncertainties of 0.1% for the electron loss correction. The one sigma uncertainties of the MC calculations are less than 0.004%.

Figure 4.21: Electron loss correction A_{eloss} and scatter correction A_{scat} as a function of tube potential for the LEES irradiated with a Philips MCN-101 x-ray tube. Added filtration is 0.2545 mm of Al. Solid symbols correspond to values derived from the measurements by Ritz¹²³ and open symbols to MC calculated values.

Impact of f_{EII} on A_{scat} and A_{eloss} : Fig. 4.22 shows A_{eloss} calculations with different f_{EII} values. The scaling of the tungsten L-shell EII cross-sections has a very small

effect on A_{eloss} which can be observed at higher energies, where this correction becomes non-unity. As the scaling factor increases, the beams become softer due to increased contribution from the L-shell. Consequently, more low-energy electrons are created in the sensitive volume and thus, fewer electrons reach the FAC electrodes before depositing all their energy. The largest effect is seen at 80 kV between the $f_{\text{EII}} = 1.0$ and $f_{\text{EII}} = 2.6$ calculations and is about 0.03% and is thus negligible.

Figure 4.22: Effect of scaling the tungsten L-shell EII cross-sections on A_{eloss} as function of tube potential for the LEES irradiated with a Philips MCN-101 x-ray tube with added filtration of 0.2545 mm of Al

The effect of scaling the tungsten L-shell EII cross-sections on A_{scat} is shown in Fig. 4.23. In this case a slight systematic increase in A_{scat} is observed with increasing scaling factor despite the data being somewhat noisier than for A_{eloss} . The largest difference is seen between the $f_{\text{EII}} = 1.0$ and $f_{\text{EII}} = 2.6$ calculations and is about 0.03% and is also negligible.

4.6. LEES CORRECTION FACTORS

Figure 4.23: Effect of scaling the tungsten L-shell EII cross-sections on A_{scat} as function of tube potential for the LEES irradiated with a Philips MCN-101 x-ray tube with added filtration of 0.2545 mm of Al

4.6.3.1 Mammography beam qualities

A comparison between MC calculated values (open symbols) and experiment based values (closed symbols) for A_{scat} (diamonds) and A_{eloss} (circle) is shown in Fig. 4.24. A similar level of agreement for A_{scat} and A_{eloss} as for the lightly filtered beam qualities is observed. Again, the MC calculated scatter correction is systematically about 0.1% higher and the correction for electron loss is unity for the entire energy range. No effect on either of these corrections was found when scaling the tungsten L-shell EII cross-sections.

Figure 4.24: Comparison of MC calculated values of the LEES FAC correction factors A_{scat} and A_{eloss} for mammography beam qualities with the values currently in use at our lab for routine calibration. A Philips MCN 101 x-ray tube with an added molybdenum filtration of 0.064 mm is used to produce these x-ray beams. Open symbols are the MC calculations and solid symbols the experimental values.

4.6.4 Correction for aperture leakage A_{ap}

The aperture correction, A_{ap} , becomes significant (larger than 0.1%) at tube potentials above 250 kV. At low energies, this correction is negligible (less than 0.025% effect) although an increasing trend towards higher energies can be seen in Fig. 4.25. A_{ap} is larger for the harder mammography beams as there should be more Compton interactions with the HEVIMET aperture for these beam qualities. No effect on A_{ap} due to changes in the tungsten L-shell EII cross-sections is observed.

Figure 4.25: Calculated aperture correction A_{ap} for the LEES irradiated by a Philips MCN 101 x-ray tube for beam qualities with 0.2545 mm Al (open symbols) and with 0.064 mm Mo (solid symbols) filtration respectively.

4.6.5 Correction for backscatter A_b

A_b , the correction factor for backscattering into the scoring field in the absence of the FAC, is found to be non-negligible in the low-energy range. This correction is about 0.65% for a 10 kV lightly filtered x-ray beam and 0.35% for the 80 kV beam. The solid circles in Figure 4.26 show how this correction varies with tube potential for the lightly filtered beams. Note that A_b^{-1} and not A_b is shown in the graph. For the harder mammography beam qualities (open diamonds) this correction is slightly smaller (about 0.4% effect) although non-negligible as well. For its relatively large contribution, this correction will change significantly the overall correction A_{total} and should be included among the corrections in the low-energy region in order to accurately extract the kerma free in air from the FAC reading. No effect on A_b due to changes in the tungsten L-shell EII cross-sections is observed.

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Figure 4.26: Inverse of backscatter correction A_b for the LEES FAC irradiated by a Philips MCN 101 x-ray tube for low-energy x-ray beam qualities with 0.0640 mm Mo (open symbols) and 0.2545 mm Al filtration (solid symbols).

4.7 Total FAC correction factors

In the preceding sections, some of the newly added corrections were found to be non-negligible depending on the energy range and beam quality. From all the corrections introduced in this work, only A_{att} , A_{scat} and A_{eloss} are applied to the NRC primary standard. Most of the other corrections are unity in the medium energy range. Except A_{ap} , which becomes relevant over 200 kV and should be taken into account (see Fig. 4.6, page 74). A comparison of the combined effect of A_{att} , A_{scat} and A_{eloss} (triangles) with the total correction A_{total} (circles) can be seen in Fig. 4.27. The difference between the two data sets is basically given by the aperture correction A_{ap} and goes from being 0.03% at 120 kV to 0.12% at 250 kV. Experimental values are also included in this figure (squares). The differences with the MC calculations reflect the discrepancies in the corrections for scatter A_{scat} and electron loss A_{eloss} (see Fig.

Figure 4.27: Comparison of MC calculated values of the MEES FAC combined correction $A_{att,exp} A_{scat} A_{eloss}$ for medium-energy Cu filtered beam qualities with the values currently in use at our lab for routine calibration. Also shown is the MC total correction factor A_{total} . The uncertainty in the total measured correction is about 0.17% (type A and B). The statistical uncertainties in the computed values for the combined correction $A_{att,exp} A_{scat} A_{eloss}$ and the total correction A_{total} are better than 0.005% .

4.4, page 70). At 120 kV, an overestimation of about 0.09% of the experimental value is observed while at 250 kV the MC calculation underestimates the experiment by about 0.05%. The conservative uncertainty assigned to these corrections seems to be an attempt to compensate for not including such effects as leakage (A_{ap}) and possible systematic uncertainties introduced in A_{scat} and A_{eloss} by the use of experimental data from a limited set of beam qualities to extrapolate these corrections for an arbitrary beam quality.

The total correction as currently used at NRC (squares) is compared with MC values (triangles) in Fig. 4.28 for the low-energy lightly filtered x-ray beams using a scaling factor f_{EII} of 1.8. Note that the MC calculated $A_{att,exp}$ has been used as

4.7. TOTAL FAC CORRECTION FACTORS

opposed to the direct MC value of A_{att} . An excellent agreement within the statistical and experimental uncertainties can be seen in the whole energy range. The almost perfect agreement at 10 kV and 15 kV seems to be a fortuitous cancellation of the $A_{\text{att,exp}}$ underestimation with the A_{scat} overestimation of the experimental values at these energies.

Figure 4.28: Comparison of MC calculated values of the LEES FAC combined correction $A_{\text{att,exp}} A_{\text{scat}} A_{\text{eloss}}$ for lightly filtered beam qualities with the values currently in use at our lab for routine calibration. Also shown is the MC total correction factor A_{total} which includes the backscatter correction A_{b} . MC values shown are for a tungsten L-shell EII cross-sections scaling factor of 1.8. The uncertainty in the total measured correction is about 0.22% (type A and B). The statistical uncertainties in the computed values for the combined correction $A_{\text{att,exp}} A_{\text{scat}} A_{\text{eloss}}$ and the total correction A_{total} are mostly better than 0.010% .

The most significant departure from a $A_{\text{att}} \cdot A_{\text{scat}} \cdot A_{\text{eloss}}$ correction at low-energies will be the inclusion of the correction for backscatter A_{b} . As demonstrated in section 4.6, this correction is over 0.4% for both sets of beam qualities in the low-

4.7. TOTAL FAC CORRECTION FACTORS

energy range and can be as large as 0.65% for a 10 kV x-ray beam. The correction for the inconsistency of the evacuated-tube technique A_x will also introduce a significative change in the total correction. While A_x is as large as 1.1% for the 10 kV beam, it is about 0.2% for the rest of the energies.

The circles in Fig. 4.28 represent the total correction A_{total} needed according to the self-consistent derivation of the FAC corrections previously introduced in section 4.1. These values will increase the needed correction (make it smaller than unity) by about 0.55% at 80 kV (0.38% from A_b and 0.19% from A_x) and by about 1.8% at 10 kV due to a 1.1% reduction from A_x and a 0.65% reduction from A_b compared to just the product $A_{\text{att}} \cdot A_{\text{scat}} \cdot A_{\text{eloss}}$. Above 20 kV the total correction is about 3% to 4% increasing to 18% at 10 kV.

A comparison of the combined effect of the attenuation, scatter and electron loss correction between MC calculated values and those in use at our lab are presented in Fig. 4.29 for the mammography x-ray beams. The agreement is within the reported experimental error of 0.22% one sigma uncertainty. The largest difference can be found at 23 kV where a 0.1% overestimation of A_{att} and A_{scat} can be seen in Figs. 4.19 and 4.24 respectively. For these beams the total correction A_{total} implies corrections from around 1.9% at 23 kV to 1.6% at 50 kV. The difference observed with the product $A_{\text{att,exp}} A_{\text{scat}} A_{\text{eloss}}$ is solely due to the 0.4% A_b correction.

4.8 Discussion of the tungsten L-shell EII cross-sections scaling factor

The need to scale the tungsten L-shell EII cross-sections to account for the significant deviation of the calculated $A_{\text{att,exp}}$ values from the measured data for the

4.8. DISCUSSION OF THE TUNGSTEN L-SHELL EII CROSS-SECTIONS SCALING FACTOR

Figure 4.29: Comparison of MC calculated values of the LEES FAC combined correction $A_{att,exp} A_{scat} A_{eloss}$ for mammography beam qualities with the values currently in use at our lab for routine calibration. Also shown is the MC total correction factor A_{total} which includes the backscatter correction A_b . MC values shown are for a tungsten L-shell EII cross-sections scaling factor of 1.8. The uncertainty in the total measured correction is about 0.20% (type A and B). The statistical uncertainties in the computed values for the combined correction $A_{att,exp} A_{scat} A_{eloss}$ are less than 0.010% and less than 0.015% for the total correction A_{total} .

lightly filtered beams deserves some discussion. K-shell EII cross-sections calculated by Kawrakow⁸¹ have been extensively benchmarked with experimental data. For instance, the K-shell EII cross-sections for Cu and Au are compared with experimental values and other theoretical and empirical models in Fig. 2.3 on page 25. Kawrakow's model matches the experimental values better than the other models, in excellent agreement within the experimental uncertainties. A similar level of agreement has been reported for Al and Ag elsewhere.⁸¹ As pointed out in section 2.3.3, this model produces shell-wise differential electron inelastic scattering-cross sections that reproduce the stopping power formula in its applicability range.

4.8. DISCUSSION OF THE TUNGSTEN L-SHELL EII CROSS-SECTIONS SCALING FACTOR

Measured tungsten L-shell EII cross-sections data are much more scarce. They are often associated with very large uncertainties, which makes them unreliable for any assessment of the accuracy and shortcomings of the different calculational models. Measured and calculated data for EII cross-sections reported in the literature were reviewed in detail by Powell¹⁴⁰ in 1976. Experimental measurements of the total ionization cross section have been performed by numerous groups since the early 1930's. However, there are only three studies of the L-shell ionization by low-energy electron impact for tungsten.¹⁴¹ Carvalho *et al.*¹⁴² measured L-subshell ionization cross-section ratios $\sigma_{L_3}/\sigma_{L_2}$ and $\sigma_{L_2}/\sigma_{L_1}$ in the energy range from 12.5 keV to 40 keV. Salgueiro *et al.* measured the ratio $\sigma_{L_3}/\sigma_{L_2}$ in the energy range from 11.59 keV to 11.98 keV. The measurements by Chang¹⁴³ from 1979 are the only available absolute measurement of the ionization cross-section of the tungsten L-subshells $\sigma_{L_1}, \sigma_{L_2}$, and σ_{L_3} . Chang used thick targets of tungsten to extract the relative ionization cross-sections from measured x-ray production cross-sections. The latter were scaled according to a scaling by McGuire,¹⁴⁴ using the value for 40 keV electrons.

Recently, Bote and Salvat¹⁴⁵ published an extensive comparison of theoretical calculated EII cross-sections with experimental values. These authors combined a relativistic plane-wave Born approximation (PWBA) model at energies above 16 times the ionization energy of the shell, U , with a semi-relativistic distorted-wave Born approximation (DWBA) below $16U$ to calculate the total EII cross-sections for L shells and K and M sub-shells of neutral atoms in a very wide energy range. The DWBA model considers the distortion of the projectile wave functions by the field of the target atom (Coulomb effect) and electron exchange between the incident and the bound electron (exchange effect). Fig. 4.30 compares the cross-section values for the three L-subshells calculated by Kawrakow, used by default in EGSnrc, with the values from Bote and Salvat and the experimental data from Chang. As can be seen, Bote and Salvat's values predict significantly higher values than Kawrakow's calculations. The

4.8. DISCUSSION OF THE TUNGSTEN L-SHELL EII CROSS-SECTIONS SCALING FACTOR

comparison with the experimental data is not conclusive due to the large uncertainties. Besides, Chang used a scaling law from a simple Born approximation calculation which reportedly disagreed with experimental values because structure effects were ignored. The relative difference of the EGSnrc tungsten L-shell EII cross-sections values with the DWBA results are shown in panel (d) of Fig. 4.30. In the energy range of interest, differences between a factor of 2.5 and 1.5 can be observed. Differences of this magnitude have been reported elsewhere in the literature. An underestimation by about a factor of 2 of the tungsten L-shell EII cross-sections calculated by Burhop¹⁴⁶ has been suggested by Fong and Tomlin¹⁴⁷ based on their own and other experimental measurements of x-ray yields. Similarly, Brown and Gilfrich¹⁴⁸ came to the same conclusion, when they compared measured K_α and L_α intensities with those expected from an electron-transport calculation.

With the capability of using arbitrary EII cross-section data in EGSnrc, it would be interesting to compare MC calculated values of $A_{\text{att,exp}}$ using the EII data from Bote and Salvat with the measured values. While the scaling used here has been assumed energy independent, the difference of their data with the EGSnrc default values is largest at low energies, decreasing to a constant value at about 50 keV, pointing to an energy dependence in the low-energy range. Preparation of EII cross-section data for EGSnrc based on the calculations by Bote and Salvat will be the subject of future work.

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Figure 4.30: Comparison of EGSnrc L_I (a), L_{II} (b), and L_{III} (c) EII cross-sections with other theoretical and experimental values. Relative difference of EGSnrc tungsten L-shell EII cross-sections (σ_{EGSnrc}) with the values from Bote and Salvat (σ_{BS}) shown in (d).

4.8. DISCUSSION OF THE TUNGSTEN L-SHELL EII CROSS-SECTIONS SCALING FACTOR

Chapter 5

HVL calculations

The Half-Value Layer (HVL) in combination with the tube potential is the quantity widely used to characterize an x-ray beam. AAPM protocol TG-61²⁴ for kilovoltage x-ray beam dosimetry and the IAEA code of practice TRS-398¹⁴⁹ chose the HVL as the beam quality specifier and most dosimetry data provided are given as a function of the HVL and the tube potential. HVL calculations reported in the literature still show large disagreements with experimental HVL values.^{30–32,107} In their extensive work, Verhaegen *et al.*³¹ used both EGS4⁷² and MCNP⁸⁷ to model x-ray systems, but did not include electron impact ionization (EII) and Rayleigh scattering in their HVL calculations. The availability of accurate experimental HVL data¹⁵⁰ and the possibility to perform very efficient Monte Carlo (MC) calculations of x-ray systems,¹⁵¹ offers a unique opportunity to investigate the accuracy of such calculations.

Although the appropriateness of HVL as the beam quality specifier for x-ray beam dosimetry is beyond the scope of this study, attention should be drawn to the fact that HVL is not a unique quantity defining a particular beam quality. Almost any HVL can be obtained by proper combinations of tube potential and beam filtration. Other beam quality specifiers have been proposed in the literature, but have not been

adopted in practice. Ideally, the best beam quality specifier would be the actual x-ray spectrum. However, this is an impractical choice given the difficulties associated with measuring or calculating this quantity accurately. Even if the spectrum can be accurately determined, compiling dosimetry data would have to be done using a unique measure of the spectrum such as the average spectrum energy. Rosser¹⁵² provided evidence pointing to the ratio of the dose at 2 cm depth in a water phantom to the dose at 5 cm depth in the same phantom, as a much better choice than the HVL. Current codes of practice attempt to reduce the ambiguity introduced by the HVL by combining it with the tube potential.

Measured HVL values are available at NRC for a large number of beam qualities in the whole kilovoltage energy range. Beams in the medium-energy range (120 kV - 300 kV) are generated with a Comet MXR-320 x-ray tube, and in the low-energy range (10 kV - 80 kV), with a Philips MCN 101 x-ray tube. These x-ray beams are routinely used for the calibration of ionization chambers. Measurements of the HVL are performed with the NRC LEES and MEES FACs.

HVLs for seven mammography x-ray beam qualities using a molybdenum filter with a tungsten anode x-ray tube Philips MCN 101 were measured at NRC for the purpose of comparison with the same beam qualities in use at the BIPM. These beam qualities were used at the BIPM for initial studies with the aim to establish much needed reference radiation qualities for mammography x-ray beams to meet the needs of National Metrology Institutions (NMIs). A future intercomparison among NMIs and the BIPM is planned using these beam qualities since not all NMIs have x-ray tubes with a molybdenum anode. In 2009, the BIPM established four reference radiation qualities for mammography x-ray beams using a molybdenum anode x-ray tube.¹⁵³

Figure 5.1: Setup used for HVL measurements as modeled with the geometry module of the EGSnrc C++ class library, `egspp`. A BEAMnrc simulation of the x-ray system is used as a particle source.

5.1 Determination of the Half-Value-Layer (HVL).

HVL is defined as the thickness of absorbing material needed to reduce the air-kerma at a distance r from the x-ray source to half its value under “narrow beam” conditions. For low-energy x-rays, the absorbing material used is Al and for medium energy x-rays, Cu is the material of choice. HVL measurements are simulated using the EGSnrc MC simulation system. The BEAMnrc user-code is used as a source to model the x-ray system as described in section 3.1 using the setup shown in Fig. 3.2 (page 35).

5.1. DETERMINATION OF THE HALF-VALUE-LAYER (HVL).

The complete experimental setup is faithfully modeled with the geometry module of `egspp`, the EGSnrc C++ class library, including the absorber holding system and the 15 cm long brass tube for scatter reduction as illustrated in Fig. 5.1. The FAC geometry is also included in the simulations with its POM placed at the scoring plane. The air-kerma at 1 m from the source, on a 5 mm radius scoring field, and the dose deposited in the collecting volume (CV) of the FAC, as well as the required corrections are calculated. The HVL is then extracted from attenuation curves of the ratio of the air-kerma or the FAC dose with absorber to the value without absorber. The same values of the absorber thickness used in the experimental HVL determination are used in the MC calculations.

Calculations can be done with either `cavity` or `egs_fac` since both codes are equally suitable for these calculations. HVL for the medium-energy and mammography beam qualities were obtained with `cavity`. For the lightly filtered low-energy beam qualities, `egs_fac` was used to assess the effect of A_x on the HVL for the 20 kV and the 80 kV tube potentials. As demonstrated in Chapter 4, the inconsistency of the evacuated-tube technique becomes non-negligible for these beams. The use of `cavity` on the other hand, has the advantage of allowing the estimation of the x-ray spectrum at the POM. These user-codes make use of the “*forced detection*” technique described in section 2.2.6 to estimate the average air-kerma within a given scoring area. This technique is intrinsically more efficient than the kerma estimation techniques described in section 2.4.1. While in the latter techniques only photons actually crossing a plane or volume contribute to the kerma, in “forced detection” every photon aimed at the scoring field contributes to the kerma. For instance, for a 200 kV x-ray beam, the kerma estimation in `cavity` is about 6 times more efficient than the kerma estimation at a plane implemented for BEAMnrc. In addition, a HVL calculation with `cavity` or `egs_fac` also benefits from the ability to take correlations into account, which further reduces the uncertainty estimate of the ratio of two strongly

5.1. DETERMINATION OF THE HALF-VALUE-LAYER (HVL).

correlated quantities. In that case, `cavity` is 13 times more efficient than `BEAMnrc`.

Inverted attenuation curves (thickness as function of attenuation) are fitted to analytical expressions using the commercial software TableCurve 2D[®] by Systat Software Inc.(SSI). TableCurve 2D's built-in library offers 3665 linear and nonlinear models including equations that may never have been considered, from simple linear equations to high order Chebyshev polynomials. The user defines the equation type to be fitted and supplies the criteria for sorting the results by goodness of fit, standard error, maximum error, F-statistic, floating point speed, or just equation number. These analytical expressions are used to evaluate the thickness of material needed for attenuating the beam to reduce the air-kerma at 1 m by half its value without absorber. The uncertainty in the estimated HVL is derived from the 95% prediction interval computed by the fitting software. The 95% prediction interval is the Y range for a given X where there is a 95% probability that the next experiment's Y value will occur, based upon the fit of the present experiment's data. The use of the prediction interval rather than the standard error of the fit is based on the fact that one is interested in a particular value from the fit. The standard error of a fit is based upon the overall fit. It does not matter if a point is near a portion of the curve that is well characterized by the fit, or a point that is poorly characterized by the fit. The prediction interval, on the other hand, is a more localized measure of error. Points near a region of the curve strongly determined by the fit will have a slightly tighter confidence interval than those points near a region of the curve that is only weakly determined in the fit.

5.1. DETERMINATION OF THE HALF-VALUE-LAYER (HVL).

5.2 Effect of different physical processes and data sets on HVL calculations

Most of the major MC simulation systems used for modeling photon and electron transport offer nowadays a more detailed treatment of particle interactions. Users have the possibility to include physical processes such as electron impact ionization (EII), Rayleigh scattering, Compton binding corrections, the generation of K,L and M characteristic x-rays and the emission of Auger and Koster-Kronig electrons, which are relevant in the low-energy range below a few hundred kilovolts. Still, some of these processes tend to be ignored in MC calculations at these energies. Rayleigh scattering is the most commonly neglected interaction process.^{31,154} It is perceived as a wasteful use of computing resources based on the fact that no energy loss and only a small angular deflection of the photon beam is involved.

In this section, the effect on the HVL of different physical interactions and photon and bremsstrahlung cross sections is quantitatively estimated for the medium-energy range. To this effect, a base case is defined which includes binding effects in Compton scattering, electron impact ionization (EII) according to the semi-empirical theory developed by Kawrakow⁸¹ and Rayleigh scattering. The best cross sections available in EGSnrc are used: NIST tabulations of differential bremsstrahlung cross sections^{116,117} which are the basis for the ICRU-37¹¹⁸ recommended radiative stopping powers, and photo-absorption and Rayleigh scattering total cross sections from the XCOM tabulations.⁷⁷ Fig. 5.2 shows the relative difference to the base case described above for several cases in the energy range 135 kV to 200 kV. In each case, a particular process has been switched off or a different cross section has been used.

Although Rayleigh scattering does not contribute directly to the energy deposition, it does affect beam attenuation. When included in the calculations, CPU time

Figure 5.2: Relative influence of Rayleigh scattering, binding corrections and EII on MC calculated HVL. The effect of selecting different bremsstrahlung and photo-absorption cross sections is also shown. Base case includes Rayleigh, EII, bound Compton scattering, and uses the NIST bremsstrahlung cross section data base and the XCOM photo-absorption cross section compilation.

is almost twice as long as when not included. However, its omission results in a 6% over-prediction of the HVL for all investigated energies (triangles in Fig. 5.2).

The EII interaction process becomes more relevant for increasing electron energy in the energy range under study. Therefore, calculations without EII (circles in Fig. 5.2) lead to an energy dependent over-prediction of the HVL ranging between 1.5% at 135 kV and 5% at 200 kV.

Including binding effects in Compton scattering, reduces the number of Compton interactions since only interactions are allowed that give electrons enough energy

5.2. EFFECT OF DIFFERENT PHYSICAL PROCESSES AND DATA SETS ON HVL CALCULATIONS

to set them free. Consequently, the Compton cross sections is decreased, which results in less attenuation of the x-ray beam, and therefore, more material (larger HVL) is needed to reduce the kerma to half its value. This is shown by the stars in Fig. 5.2 representing the effect of neglecting binding in Compton scattering. A 1% underestimation of the HVL is observed throughout the energy range investigated.

Use of the older Storm and Israel photo-absorption cross section tabulations instead of XCOM has a relatively small effect of about 0.4% in this energy range (see squares in Fig 5.2). Bethe-Heitler bremsstrahlung cross sections are the default in EGS4 and EGSnrc. These values are based on a first Born approximation with an empirical correction factor below 50 MeV. On the other hand, the NIST bremsstrahlung cross section data base was obtained from partial wave analysis calculations below 2 MeV and constitutes the basis for the ICRU radiative stopping powers. Simulations with the Bethe-Heitler bremsstrahlung cross sections (diamonds) instead of the NIST tabulations result in softer spectra and HVL underestimation ranging between 3% at 135 kV and 6% at 200 kV.

These results show that physical processes relevant to low-energy photon interactions, as well as the most accurate cross sections must be included in MC simulation to avoid significant errors in HVL calculations. Although the combined effect of omitting all these processes and using the older data seems to mitigate this difference, it can still be as large as 3.5%.

As explained in section 2.3.2, a small, but non-negligible, sensitivity to the energy grid used for the interpolation of the photon cross section was detected. When going from a 1 keV - 20 MeV grid with 200 bins to a 1 keV - $E_{\text{max}} + 1$ keV energy grid with 20000 bins a difference in the HVL of 0.43 % is observed at 120 kV. This effect decreases with increasing energy until it becomes negligible at 300 kV within the statistical noise. The use of 20000 interpolation points here is only for demonstrative

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purposes. One can actually achieve a good interpolation accuracy with much less points. All calculations reported here were done using 2000 interpolation points.

5.3 HVL for medium energy x-ray beams

The availability of accurate experimental HVL values at our lab offers an excellent opportunity to check our ability for modeling x-ray tubes with the EGSnrc/BEAMnrc simulation system. The disagreement between measured and calculated HVLs previously reported in the literature ranges from about 2% up to more than 10%.³⁰⁻³² In their extensive work, Verhaegen *et al.*³¹ reported measured and calculated HVL in terms of mm of Cu and Al. Although no numerical comparison is tabulated in their work, one can see from the graphical comparison that the measured values are larger than those obtained from their MC calculated spectra. Relative differences for the HVL in terms of mm of Cu of a Philips MCN421 unit for the P6 (150 kV tube potential, 4Al + 1.2 Sn filtration) and the P8 (200 kV tube potential, 4Al + 2.0 Sn filtration) beam qualities are 11.0% and 6.7% respectively.

Fig. 5.3 shows a comparison of MC calculated HVLs with experimental HVLs measured at NRC for several tube potentials from 120 kV up to 300 kV. On the left side, the measured HVL (squares) is compared with the HVL computed directly using air-kerma ratios (circles), which is equivalent to correcting the FAC reading for all effects. An increasing discrepancy with tube potential can be observed. On the right side, the relative difference between experiment and the MC calculations is shown (circles). As in the work by Verhaegen *et al.*,³¹ MC calculated HVLs underestimate the ones extracted from the measurements. A minimum difference of about 1.0% is seen at 120 kV, increasing to 2.5% at 300 kV. The measured dose ratio uncertainties are of the order of 0.1%.¹⁵⁰ The statistical uncertainties of the MC calculated kerma

Figure 5.3: **Left:** Comparison of EGSnrc calculated HVL values with those from attenuation measurements performed at NRC with the MEES FAC for medium-energy beam qualities. **Right:** Relative percentage difference of the calculations with the experiment when using K_{air} ratios (triangles) or $D/A_{att}/A_{scat}/A_{eloss}$ (squares) ratios. Values reported here are first HVL in terms of mm of Cu. Uncertainties shown are based on 95% confidence level predictions from the least square fitting procedure.

ratios is better than 0.05%.

From the set of corrections defined in Chapter 4, measured attenuation curves are only corrected for attenuation, scatter and electron loss. To assess whether this has any impact on the HVL, the MC simulation includes the MEES geometry to compute the corresponding correction factors for the varying Cu absorber thickness. The MEES is positioned in such a way that the FAC's POM coincides with the position of the kerma scoring plane shown in Fig. 5.1. The results from these calculations are also included in the graph on the right side of Fig. 5.3 (triangles). Within the one sigma statistical uncertainties there is no significant difference between the two calculations. However, over 200 kV tube potential a slight difference can be observed caused by the omission of the aperture correction A_{ap} . Including A_{ap} will remove the contribution from photons leaking through or scattering at the aperture and hence the attenuation curve will be softer leading to a lower HVL. The ratio of the aperture correction A_{ap} at 300 kV for a thickness d to the value with no absorber is plotted

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Figure 5.4: Ratio of aperture correction A_{ap} for a 300 kV beam for absorber thickness d to the value without absorber as a function of thickness.

in Fig. 5.4. At around 5.5 mm, this ratio is about 1.002 consistent with the 0.19% reduction of the HVL observed on the right graph of Fig. 5.3.

Discrepancies with the experimental values cannot be explained by the small effect of ignored or differing FAC correction factors. A reduction of the photo-absorption cross section, a slight hardening of the bremsstrahlung spectrum, or a combination of the two, within the reported uncertainties of the respective cross sections,^{77,116,117,155} could account for these differences. Nevertheless, the increasing underestimation of the experimental HVL with tube potential points to a need for a hardening of the bremsstrahlung spectrum as a more likely cause of these discrepancies.

5.3. HVL FOR MEDIUM ENERGY X-RAY BEAMS

5.4 HVL for lightly filtered beam qualities

In the experimental HVL determination for low-energy beams, FAC readings were only corrected for attenuation, the largest FAC correction at these energies. The most likely explanation for neglecting corrections for scatter and electron loss is their relative insensitivity to beam quality seen in Fig. 4.21 for the values in use at our lab. HVL is calculated by modeling the measuring setup described in Fig. 5.1 together with the FAC used for these measurements, the LEES. Calculated values of the dose deposited in the LEES collecting volume (CV) for Al absorbers of varying thickness were corrected for attenuation with the MC calculated A_{att} correction factor. Fig. 5.5 shows a comparison of the MC results with the experimental values. An increasing overestimation of the experimental HVL with increasing tube potential is evident on the left side of this figure.

Figure 5.5: **Left:** Comparison of EGSnrc calculated HVL values with experimental values for the lightly filtered low-energy beam qualities obtained from attenuation measurements performed at NRC with the LEES FAC. Values reported here are first HVL in terms of mm of Al. **Right:** Plot of relative difference with experimental HVL values.

On the right side of Fig. 5.5, a quantitative measure of the discrepancies with

the experimental values is presented. At 10 kV an underestimation of about 4% can be seen. At 80 kV the calculation overestimates the experiment by as much as 31%. These differences are qualitatively very similar to the discrepancies encountered for the attenuation correction A_{att} for these beam qualities in the previous chapter. Although in this case, where attenuation is much stronger, the effect is quantitatively larger. The above observation and the increasing disagreement with increasing energies, makes the argument for a scaling of the tungsten L-shell EII cross-sections from Chapter 4 stronger. Using the line of thought from Eq. (4.31), page 81, a 31% discrepancy in the HVL can only be explained by an uncertainty in the photon cross section of the same magnitude which is unrealistic.

Following the same procedure as in Chapter 4, sets of HVL were obtained using different scaling factors f_{EII} of the tungsten L-shell EII cross-sections. The results are plotted on the left side of Fig. 5.6 together with the experimental values (squares). A scaling factor of 2.6 pushes the HVL curve too far down, and a scaling factor of 1.8 too far up. A scaling factor of 2.1 matches the experimental HVL significantly better. There is no sensitivity to the scaling factor at 10 kV, although an improvement of the order of 1% is observed on the right side of Fig. 5.6 at this energy compared to no scaling at all (see right side of Fig. 5.5). The agreement with the experiment is better than 2% for all beam qualities except at 10 kV when scaling the tungsten L-shell EII cross-sections by a factor of 2.1. The high sensitivity of the HVL to the scaling of the tungsten L-shell EII cross-sections is noteworthy and may help to explain previously reported uncertainties.

FAC readings are only corrected for attenuation during the experimental procedure to determine the HVL. This correction will decrease as more absorber material is placed in front of the x-ray beam, hardening it. For this reason, the combined effect of the scatter and electron loss corrections will be more visible with increasing tube

5.4. HVL FOR LIGHTLY FILTERED BEAM QUALITIES

Figure 5.6: **Left:** Comparison of EGSnrc calculated HVL values using different scaling factors of the tungsten L-shell EII cross-sections with experimental values for the lightly filtered low-energy beam qualities obtained from attenuation measurements performed at NRC with the LEES FAC. Values reported here are first HVL in terms of mm of Al. **Right:** Plot of relative difference with experimental HVL values.

potential. As shown in Fig. 4.21, page 95, A_{scat} is about 1.005 and A_{eloss} becomes less than unity above 50 kV with a correction as large as 0.2%. This is demonstrated in Fig. 5.7 for two values of f_{EII} , 1.8 and 2.1. For a scaling factor of 1.8 (left side), the HVL determined using D/A_{att} ratios (circles) underestimates by 0.7% the HVL obtained from K_{air} ratios (diamonds) for the 80 kV beam. However, there is a 0.4% underestimation if one uses $A_{\text{att,exp}}$ (squares) instead of A_{att} to correct the dose ratios. In the case of $f_{\text{EII}} = 2.1$, the effect of neglecting the rest of the correction factors in the HVL determination amounts to a 0.26% underestimation of the HVL for the 80 kV beam. The omission of A_{scat} and A_{eloss} or the use of only A_{att} or $A_{\text{att,exp}}$ as opposed to using all corrections have a small impact on the HVL and does not account for the large differences with the experiment.

5.4. HVL FOR LIGHTLY FILTERED BEAM QUALITIES

Figure 5.7: Relative difference of MC calculated HVL with experiment for low-energy lightly filtered x-ray beams. Calculations using K_{air} ratio curves (diamonds) and obtained from D/A_{att} ratio curves (circles) are shown for two values of f_{EII} , 1.8 (left) and 2.1 (right). The effect of using $A_{\text{att,exp}}$ rather than A_{att} is also shown for $f_{\text{EII}} = 1.8$ at 20 kV and 80 kV (squares).

5.5 HVL for mammography beam qualities

HVL values obtained for mammography beam qualities are shown on the left side of Fig. 5.8 together with the experimental values. These HVLs are larger than the values for the lightly filtered beams of same tube potential. Differences of the calculated HVL with experimental values for the mammography beam qualities are not as large as in the case of the lightly filtered beams as demonstrated on the right side of Fig. 5.8. But an increasing discrepancy with tube potential is evident reaching a value of about 2% at 50 kV.

A much better agreement with the experimental values at the 0.5% level is obtained by scaling the tungsten L-shell EII cross-sections. Values of the HVL lie much closer for different f_{EII} values than for the lightly filtered beams. At these beam qualities, no significant differences can be observed on the right side of Fig. 5.9 between using a 1.8 or a 2.1 value of the tungsten L-shell EII cross-sections scaling factor f_{EII} .

5.5. HVL FOR MAMMOGRAPHY BEAM QUALITIES

Figure 5.8: **Left:** Comparison of EGSnrc calculated HVL values with experimental values for mammography beam qualities obtained from attenuation measurements performed at NRC with the LEES FAC. Values reported here are first HVL in terms of mm of Al. **Right:** Relative difference of MC calculated HVL with experimental HVL.

Figure 5.9: **Left:** Comparison of EGSnrc calculated HVL values using different scaling factors of the tungsten L-shell EII cross-sections with experimental values for the mammography beam qualities. Values reported here are first HVL in terms of mm of Al. **Right:** Plot of relative differences with experimental HVL values.

5.5. HVL FOR MAMMOGRAPHY BEAM QUALITIES

5.6 Discussion

The disagreement found with the measured HVL for lightly filtered x-ray beams has been accounted for by scaling the tungsten L-shell EII cross-sections in the same manner as in Chapter 4. However, best agreement with experiment is only obtained with a slightly different value of the scaling factor f_{EII} . While the MC calculated attenuation correction $A_{\text{att,exp}}$ agrees better with experiment for $f_{\text{EII}} = 1.8$, a value of 2.1 is needed to match the experimental HVL values.

A value of $f_{\text{EII}} = 1.8$ is in line with the excellent agreement of the calculated $A_{\text{att,exp}}$ values for medium-energy beams, while discrepancies in the HVL of the order of 1% to 2% remain in this energy range. This would imply accepting a level of agreement in the HVL between the calculations and the measurements of 5% to 8%. Finding the proper scaling requires a detailed analysis of the combined effect of the photon cross-section uncertainties and the scaling of the tungsten L-shell EII cross-sections. These uncertainties will affect the HVL and A_{att} differently since the attenuation takes place in Al and air respectively. As mentioned in section 4.8, the impact of the EII cross-sections calculated by Bote and Salvat on the accuracy of MC simulation of attenuation experiments will have to be considered as well.

Chapter 6

Fast CBCT scatter corrections

Cone beam computed tomography (CBCT) imaging has become a valuable tool not only for patient localization, but also for dose verification. For the latter, an accurate reconstruction of the phantom is required. This accuracy can be significantly reduced by the scattered photons which reduce image contrast resolution, increase image noise and produce streak and cupping artifacts. It is therefore important to develop methods to remove the scatter signal from the scans.

In CBCT imaging, scatter corrections are commonly performed experimentally^{156–166} by increasing the object-detector air-gap, using anti-scatter grids, or combining both. These methods can reduce the scatter in some cases, but also reduce the primary signal intensity. Beam stop arrays (BSA) techniques have been shown to effectively reduce the scatter-primary ratio by a factor of 14.¹⁶³ However, BSA techniques are not practical since two acquisitions per angle are required increasing the patient dose and acquisition time. Algorithmic methods using analytical models have been also used which are fast,^{167,168} but are of limited use when complex geometries or heterogeneous media are involved.

The most accurate method available for scatter correction in CBCT is to calculate the scatter using a Monte Carlo (MC) simulation.^{169,170} The photon scatter model used in the simulation should be accurate enough so that no significant bias is introduced in the reconstructed image.^{171,172} Since the variance per incident particle is much larger for the scatter signal compared to the primary signal, prohibitively long calculations are required in order to achieve a desired statistical precision if no special techniques are used. Hence it is also necessary to implement efficient algorithms that reduce CPU time to a practical level for clinical use within a desired statistical uncertainty without loss of accuracy.

In recent years, several authors have published efficient MC algorithms for CT scatter corrections.^{68–70,170,173,174} Zbijewski and Beekman⁶⁹ proposed a modified point detector method combined with a 3D Richardson-Lucy fitting algorithm for scatter correction of small animal CBCT scans. Efficiency gains of about 4 orders of magnitude were reported by these authors. The fitting algorithm exploits the assumption of a smooth scatter distribution in each projection and between neighboring projections which is acceptable for small animal CBCT with scatter-to-primary-ratios (SPRs) of 20%. However, SPRs in excess of 100% have been reported in the literature¹⁷⁵ for a human pelvis phantom.

Poludniowski *et al.*⁷⁰ proposed a coarse reconstruction fixed detection (CRFD) algorithm for scatter correction in kV CBCT. In this approach only a small number of detector nodes were used combined with a reduced number of projections. A linear interpolation between nodes and projections is used to extract the scatter distribution for a desired scan configuration. This approach also relies on the smoothness of the scatter distribution in each projection and between projections. In situations where the smoothness assumption fails, linear interpolation might not be adequate for accurately reproducing the scatter distribution. The scatter distribution of a

water sphere irradiated by 60 keV photons is shown in the left panel of Fig. 6.1. Double rings due to inclusion of molecular effects can be observed in this particular simulation. The central profile of the scatter distribution is plotted on the right panel, clearly showing high frequency peaks near the edge of the phantom due to Rayleigh scattering. These would be missed if an interpolation grid is used that is too coarse.

Another issue with using approximations of this kind is the fact that even for smooth scatter distributions, there may be regions of high SPRs where accurate knowledge of the scatter signal is very important. Wiegert¹⁷⁶ showed that the SPRs of a head phantom can vary strongly for individual projections thus causing the relative impact of the scatter to be locally strongly varying.

In this Chapter, several VRTs are described in detail which improve the efficiency of the estimation of the photon scatter contribution to a CBCT scan by several orders of magnitude compared to analog calculations (no VRT). No *a priori* assumptions are made about the scatter distributions and the CBCT setup is faithfully modeled. The effect of the different VRTs on the calculation efficiency of the scatter distribution is discussed. Special attention is paid to the `splitting + RR` techniques which have the largest impact on the efficiency.

To accelerate the scatter calculations even further, simpler physical scatter models could be used. As long as the scatter distribution produced by this simpler model is similar in shape to the actual scatter distribution, one could use it to successfully remove the scatter from the scan. However, care must be taken that no significant bias is introduced by these simplifications. An accurate way to assess whether a specific scatter model is suitable for a scatter correction algorithm requires a complete implementation of the algorithm. Section 6.4 introduces a CBCT scatter correction algorithm and demonstrates its ability to accurately reproduce several test phantoms. The impact of smoothing the scatter distribution on the correction algo-

rithm is discussed in sections 6.5.1 and 6.6.2. Finally in section 6.7, different physical scatter models are used to study their effect on the accuracy of the reconstruction process.

Figure 6.1: **Left:** Scatter distribution of a 30 cm diameter water sphere. **Right:** Central horizontal profile from the scatter distribution.

6.1 Details of the MC calculation

A new EGSnrc²² user-code, `egs_cbct`, is developed for the purposes of this investigation. `egs_cbct` is written in C++ and uses the EGSnrc C++ class library `egspp`.⁷⁶ Air-kerma at the detector plane is scored efficiently using a track-length estimation, whereby all photons crossing the scoring plane contribute to the kerma. This has been shown in Fig. 2.5, page 29, to be about 20 times more efficient than computing kerma by switching off electron transport and collecting the energy deposited by electrons on the spot. In addition to the CBCT scan, this user-code can generate the individual components of the CBCT scan, i.e., primary (attenuated) and scatter signals. A “measured” scan is obtained from a lengthy calculation to reduce the statistical noise as much as possible. On average the statistical uncertainty of the “measured”

scans was not more than 0.2 %. Photons are simulated down to 1 keV and electron transport is turned off by setting ECUT, the electron transport cut-off, higher than the maximum photon energy used in the calculations. The state-of-the-art photon cross-section compilation XCOM¹¹⁹ is used in the calculations. Coherent scattering (Rayleigh) is simulated using the Independent Atom Approximation (IAA) as inherited from EGS4⁷² and incoherent scattering (Compton) is modeled in the relativistic impulse approximation (RIA) taking into account binding and Doppler broadening.⁹⁴ Photons undergoing photoelectric absorption are immediately terminated.

CBCT scans and their corresponding primary and scatter contributions are estimated for several phantoms irradiated by either a 120 kV x-ray beam or a monoenergetic 60 keV photon beam. These beams are modeled as a point source located at 100 cm from the phantom's center. A detector is centered at 155 cm from the source along the line connecting the source with the phantom's center. The source-detector system can be rotated around the phantom in a similar fashion as during the acquisition of a CBCT scan. In this work, we chose to use an isotropic point source irradiating only a certain area or solid angle (**collimated source**). The source target shape is a square of fixed size insuring the beam covers the whole detector area. The same number of particle histories was run for all projection angles.

The central point in this work is improving the calculation efficiency of the scatter contribution from the phantom. For the sake of simplicity we assume an ideal detector of 100% detection efficiency. With this assumption, the detector can be modeled as a simple square surface divided into $N \times N$ smaller squares (pixels). For realistic systems the actual details of the detection system need to be included in the calculations. Moreover, the detector's output is considered to be proportional to the energy deposited per unit mass as is the case for ionization chambers. From these two assumptions it is clear that one needs to implement an algorithm that efficiently

6.1. DETAILS OF THE MC CALCULATION

estimates the air-kerma due to scattered photons K_{scat} at the detector. In the case where the detector signal may be proportional to either the photon fluence (photon-counting detectors) or the photon energy fluence (scintillation detectors), one will have to optimize the algorithm for these quantities instead.

Efficiency is calculated using the expression

$$\varepsilon = \frac{1}{RMSE^2 \cdot T_{CPU}}, \quad (6.1)$$

where $RMSE$ is the relative root mean square error of the scatter signal and T_{CPU} is the CPU time of the calculation. RMSE is defined here as follows

$$RMSE = \left(\frac{1}{N} \sum_{i=1}^N \frac{\Delta x_i^2}{x_i^2} \right)^{\frac{1}{2}}, \quad (6.2)$$

where x_i and Δx_i are the value of the signal and its estimated uncertainty in pixel i respectively, and N the number of pixels with non-zero signal.

6.2 Implemented variance reduction techniques

Several VRTs are combined in `egs_cbct` in order to increase the efficiency of scatter estimation in CBCT scans. The *forced detection* technique (FD), described in section 2.2.6 is used to compute the contribution from all photons aimed at the scoring field without having to wait until they reach the detector, allowing a more efficient sampling of all possible contributions. A further increase in efficiency is obtained by means of the mean free path transform (*MFPTR*) from section 2.2.7. This technique produces more interactions deeper in the phantom (path stretching), from where more contributions to the scatter signal come, without exhibiting a dependency on the particle's direction. This transformation reduces weight fluctuations and therefore has

a reduced variance associated with it. Photons not moving towards the detector, i.e., their direction does not intercept with the detector, are transported using *Woodcock tracing* (see 2.2.8) to minimize the time spent transporting photons that are less likely to contribute to the signal.

A combination of *interaction splitting* with *Russian Roulette* (RR) is developed that not only increases the number of scoring particles but also makes sure the particles' weights or contributions to the signal are nearly constant, which leads to a considerable reduction of the variance of the scored quantity. Different approaches are explored for selecting the splitting numbers:

1. Fixed splitting (FS)
2. Position dependent importance splitting (PDIS)
3. Region dependent importance splitting (RDIS)

Because of their great impact on the efficiency, they are described below in more detail.

6.2.1 Fixed splitting (FS) and constancy of weights.

In the initial implementation of the `splitting + RR` technique, splitting numbers for primary photons N_p and for secondary photons N_s are set to constant values. A diagram describing this technique is shown in Fig. 6.2. After transporting the photon a distance λ_1 to the interaction point, the interaction is split resulting in N_p scattered photons with a weight of wt_0/N_p , where wt_0 is the initial weight. These photons are either normally incorporated into the shower without any further splitting, if they are aimed at the detector (solid arrows), or killed by RR with a probability $1 - 1/N_s$, if they are moving away from the detector (crossed out dotted arrows). A photon

Figure 6.2: Diagram describing the fixed splitting technique. A photon interaction is split N_p times at λ_1 and those photons not aimed at the detector are killed with probability $1 - 1/N_s$ (crossed-out dotted arrows). A photon surviving the RR game with weight $wt_0 \cdot N_s/N_p$ (dot-line arrow) interacts at λ_2 and the same procedure is repeated for the second-order scatter but splitting the interaction N_s times. All photons contributing to the detector signal have the same constant weight wt_0/N_p .

surviving the RR game carries a weight $wt_0 \cdot N_s/N_p$ (dot-line arrow). To avoid the detrimental effect of varying weights on the variance, when the photon surviving the RR game arrives at the interaction point λ_2 , its interaction is split N_s times and the same procedure is applied to these second order scattered photons. This approach guarantees that the resulting photons will have the same weight as the photons aimed at the detector. Initial photons not aimed at the detector survive RR with a probability N_p/N_s and the interaction of surviving photons are split N_s times thus making sure their weight is also wt_0/N_p . Optimum values for N_p and N_s can be found by performing short runs for a desired setup with varying splitting numbers.

6.2. IMPLEMENTED VARIANCE REDUCTION TECHNIQUES

6.2.2 Position dependent importance splitting (PDIS).

The above procedure for selecting the splitting number N_p can be modified so that this time not the weights of the particles but their contribution to the detector signal is nearly constant. This way, a significantly larger reduction of the variance can be achieved. The splitting number N_p^i must be obtained before the interaction takes place. It is calculated from the ratio of the potential signal from the i -th particle's interaction site K_a^i , to the average primary signal on the detector, $\bar{K}_a$, times an adjustable parameter f_{split} ,

$$N_p^i = wt_i \cdot \frac{K_a^i}{\bar{K}_a} \cdot f_{\text{split}}, \quad (6.3)$$

where wt_i is the i -th particle's weight and K_a^i is the air-kerma that would be contributed to the signal from the interaction site if the particle did not interact. The attenuation is done here for a user-defined medium which should be the most abundant medium in the phantom. The attenuation path goes either along the particle's direction if it is aimed at the detector or along the scoring plane's normal if it is not directed at the detector. $\bar{K}_a$ is selected for being a quantity with negligible uncertainty. With this prescription, all photons contributing to the detector signal will have a weight

$$wt_i = \frac{1}{f_{\text{split}}} \cdot \frac{\bar{K}_a}{K_a^i}, \quad (6.4)$$

and the value of the scoring signal will be

$$wt_i \cdot K^i = \frac{\bar{K}_a}{f_{\text{split}}} \cdot \frac{K^i}{K_a^i}, \quad (6.5)$$

which will approach the constant value $\bar{K}_a/f_{\text{split}}$ the more similar K^i , the air-kerma after the interaction, is to K_a^i . In this fashion nearly constant contributions from all particles and consequently a great reduction of the variance are obtained. However, since K_a^i is computed before the interaction takes place, the actual contribution af-

ter the interaction K^i can be different due to energy loss and or direction change. Moreover, the attenuation for K_a^i is for a homogeneous medium which could be very different from the actual attenuation of the photon on its path to the detector.

A RR game is played with photons not aimed at the detector after the interaction in the same fashion as in section 6.2.1. The only difference here is that photons surviving RR will be split according to the prescription from Eq. (6.3) which can be easily shown to produce the scoring signal from Eq. (6.5).

Similar to Fixed Splitting (FS), this more sophisticated technique requires only 2 parameters to be optimized, namely f_{split} and N_s . Moreover, to compute K_a^i , one needs to ray-trace the path from the interaction point to the detector.

6.2.3 Region dependent importance splitting (RDIS).

Another approach for selecting the splitting number N_p is to divide up the phantom into importance regions. The importance C_j of such a region is calculated as the ratio of the average contribution from region j to the signal, $\bar{K}_j$, to the average contribution from all regions to the signal, $\bar{K}$. The splitting number N_p^i for the i -th photon in region j is selected according to the following prescription

$$N_p^i = wt_i \cdot C_j \cdot N_p \quad \text{with} \quad C_j = \frac{\bar{K}_j}{\bar{K}}, \quad (6.6)$$

where wt_i is the i -th particle's weight. With this prescription, all photons will have a weight

$$wt_i = \frac{1}{C_j \cdot N_p} = \frac{1}{N_p} \cdot \frac{\bar{K}}{\bar{K}_j}, \quad (6.7)$$

which is constant in a given importance region, and their contribution to the detector will therefore be

$$wt_i \cdot K_j^i = \frac{\bar{K}}{N_p} \cdot \frac{K_j^i}{\bar{K}_j}, \quad (6.8)$$

and since the value of K_j^i , the air-kerma delivered by a particular photon from the importance region j will be relatively similar to $\bar{K}_j$, one will achieve nearly constant contributions from all particles thus greatly reducing the variance.

A RR game is played in the same fashion as in section 6.2.1 but with the difference that the splitting number for photons surviving RR is selected according to Eq. (6.6) so that their contribution to the detector is also given by Eq. (6.8).

To avoid very large and very small splitting numbers in the early stages of the simulation (when the uncertainties in $\bar{K}_j$ are large), minimum and maximum splitting number cutoffs $N_{\min}$ and $N_{\max}$ are needed. A so called “warming” period is also needed at the beginning during which all importances are set to unity and therefore the splitting scheme reverts to the FS technique. The proper length of this “warming” phase must be investigated. The longer this phase, the smaller the uncertainties of the initial importances. However, too large “warming” phases will also have a detrimental effect on the efficiency due to prolonged CPU time. In this work, the first 10 % of all the histories are used for the “warming” phase. The values of $\bar{K}_j$ and $\bar{K}$ are accumulated during the simulation and the importances are updated periodically after 10 % of the histories have been executed. The central slice of the importance map of the water phantom with bone inserts is shown on the left side of Fig. 6.3. The beam is incident from the left. Darker values correspond to lower values of the importance. One can see how in the regions with bone the importances are reduced due to increased attenuation. The importance increases for regions near the bottom of the phantom (to the right of the image) from where scattered particles are more likely to reach the detector. This is better seen on the right side of Fig. 6.3

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where the central importance profile is compared to a profile between the upper bone inserts.

Figure 6.3: **Left:** Central slice of the importance map for the $60 \times 60 \times 60$ water phantom with 5 bone inserts irradiated from the left with 120 kV x-rays. **Right:** Importance profiles along the central line and for a line between the two upper bone inserts.

RDIS requires the optimization of 2 more parameters than FS and PDIS. Besides N_p and N_s , one needs to find optimum values for $N_{\min}$ and $N_{\max}$.

6.2.4 Smoothing the scatter distribution.

To further decrease the simulation time, the scatter scan $\tilde{S}_i$ is subjected to smoothing using a 2D version of the acLASG filter developed by Kawrakow¹⁷⁷ to smooth MC calculated dose distributions for use in RTP. Due to the fact that in general the scatter distribution is a “well behaved” function without sharp discontinuities, the denoising algorithm performs very well. This is illustrated in Fig. 6.4 for a simple homogeneous water cylinder with the x-ray source rotating around the symmetry axis.

Figure 6.4: Comparison of the scatter distributions from calculations with a negligible uncertainty (black line), a large statistical uncertainty obtained in 15 seconds of CPU time (red symbols) and the fast calculation after denoising (blue line) for a simple homogeneous water cylinder irradiated with a 60 keV photon beam.

6.3 A word on image reconstruction algorithms.

Initially the filtered back-projection (FBP) algorithm due to Feldkamp, Davis and Kress¹⁷⁸ (FDK) was used which is both fast and reported to be relatively accurate. The switch to a statistical reconstruction method in the last stage of this study was motivated by the fact that the FDK algorithm was not as accurate reproducing a head phantom as it was when used for reconstructing a spherical phantom. A modified version of the Maximum Likelihood Expectation Maximization (MLEM) reconstruction algorithm¹⁷⁹ known as the Ordered Subsets Expectation Maximization (OSEM)¹⁸⁰ was used which improves convergence speed over the MLEM approach and is more accurate than the FDK algorithm. Differences between the reconstructed and original spherical phantom using a scatter-free scan with the FDK algorithm were about 2 % to 3 % depending on the number of projections used. However, in the head phantom case this difference was as large as 6 %. The OSEM algorithm is capable

of reproducing the original phantom at the 2.5 % level with one iteration and at the 1.2 % level with 3 iterations. All differences reported above were calculated as the Mean Absolute Percentage Error (MAPE) defined in section 6.3.1 below. Statistical reconstruction methods are more accurate than FBP algorithms, although accuracy comes at the price of increased CPU time.

6.3.1 Measuring image reconstruction accuracy.

The agreement of the estimated image with the original image can be measured directly by comparing the estimated phantom with the original phantom or indirectly by comparing a scan of the estimated phantom with the “measured” scan. Although mostly phantom comparisons will be shown here, scan comparisons in the initial stage (spherical water phantoms) are also shown for illustrative purposes. It is obvious that in real clinical situations one does not dispose of the original phantom. Hence, a scan comparison is a practical way to set a convergence criterion.

The Relative Root Mean Square Error (RMSE) is commonly used as a measure of the predictive power of an algorithm. It is defined here as follows

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N \frac{(x_i - x_i^o)^2}{x_i^o{}^2}}, \quad (6.9)$$

where x_i and x_i^o are the estimated and reference value in voxel/pixel i respectively, and N the number of phantom voxels or scan pixels depending of whether one is comparing phantoms or scans. Mathematically, the RMSE is always positive, resembling a distance, thus indicating how close the estimated value is from the real value. However, because of the squaring of each term in the sum, it is very sensitive to outliers effectively weighting large errors more heavily than small ones.

This property of the RMSE has led researches to use a quantity less sensitive

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to outliers, the Mean Absolute Percentage Error (MAPE). It is defined as

$$MAPE = \frac{1}{N} \sum_{i=1}^N \left| \frac{x_i - x_i^o}{x_i^o} \right|, \quad (6.10)$$

with the quantities on the r.h.s. of the equation having the same meaning as in Eq. (6.9). A disadvantage of both, the RMSE and the MAPE, is the possibility of having reference values of zero, in which case there will be a division by zero in Eq. (6.10). Moreover, because they take only positive values without upper bound, they are prone to right-skewed asymmetry.

If one is interested in following the trend of the algorithm, one can use the Mean Relative Error (MRE), which is a signed measure of the error. This quantity indicates whether the estimated values are biased, i.e., whether they tend to be disproportionately positive or negative. However, the MRE can be misleading in cases of large positive and negative errors canceling out, producing a relatively small mean value. MRE is defined as

$$MRE = \frac{1}{N} \sum_{i=1}^N \frac{x_i - x_i^o}{x_i^o}. \quad (6.11)$$

Under the assumption that the individual relative errors are not correlated, the RMSE and MRE of an estimator are related by the expression

$$RMSE^2 = \sigma^2 + MRE^2 \quad (6.12)$$

where σ^2 is the underlying variance of the distribution of relative errors. One can appreciate the value of the RMSE as an overall measure of the error since it includes both, the bias (accuracy) and the spread (precision) on the estimated values. These two quantities (RMSE and MRE) will be used in section 6.7 to evaluate the accuracy

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of the different photon scatter models.

6.4 Scatter correction algorithm.

6.4.1 Definitions

A CBCT scan consists of a set of projections onto a 2D detector array around the volume of interest in a 180° or 360° orbit. If R_i denotes the reading in pixel i for a given projection and S_i the corresponding scatter contribution to the signal, then the quantity

$$a_i = \ln \frac{b_i}{A_i} = \ln \frac{b_i}{R_i - S_i} = \int \mu(l) dl \quad (6.13)$$

is the attenuation along a line connecting the x-ray source with the detecting element i . The blank scan b_i is the signal at pixel i without the phantom and μ is the attenuation coefficient at position l along the line. If the scatter contribution S_i is known, then the scatter-free scan a_i (or A_i) can be computed according to Eq. (6.13) and given to an image reconstruction algorithm to obtain the 3D distribution of attenuation coefficients in the phantom. The quantity actually measured by the scanner is

$$r_i = \ln \frac{b_i}{R_i}. \quad (6.14)$$

In what follows $s_i = S_i/b_i$ is a short hand notation and symbols with a tilde denote MC computed quantities, *e.g.* $\tilde{r}_i$ is the real scan obtained from the MC simulation, $\tilde{S}_i$ the scatter, etc. Because the main purpose of this investigation is to assess VRT in the MC simulation and the iterative scatter correction algorithm described in the next section, only scans generated by a MC simulation are used in this paper, a very simple x-ray source is employed (a monoenergetic 60 keV point source) and the detector response is assumed to be given by air-kerma. Use of measured scans, a realistic

photon source, and a realistic detector response is left for future investigations.

6.4.2 Iterative scatter correction algorithm

The proposed iterative scatter correction algorithm works as follows:

1. Set $a_i = r_i$
2. Reconstruct the phantom using the current estimate of a_i . Either an FDK filtered back-projection algorithm or an iterative OSEM algorithm can be used in this step.
3. Compute the scatter-free scan $\tilde{A}_i$ and the scatter $\tilde{S}_i$ corresponding to this phantom
4. Perform a scatter correction. The first approach considered is

$$a_i = (1 + \alpha)r_i - \alpha\tilde{r}_i - \ln \frac{\tilde{A}_i}{\tilde{A}_i + \tilde{S}_i} \quad (6.15)$$

with α a relaxation parameter. The second approach is defined via

$$a_i = r_i - \ln \left[1 - \tilde{s}_i \exp(\beta r_i + (1 - \beta)\tilde{r}_i) \right] \quad (6.16)$$

with β a free parameter.

5. Go to step (2).

The iteration is stopped when convergence has been reached, with a suitable termination criterion currently under investigation. In all examples presented in this thesis a manual inspection after each iteration is used.

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Eq. (6.15) is easily obtained from Eq. (6.13) by replacing A_i with $\tilde{A}_i \cdot R_i/\tilde{R}_i$, assuming that major differences in R_i and $\tilde{R}_i$ are given by differences in their attenuation properties. Finally a relaxation term $\alpha \cdot (r_i - \tilde{r}_i)$ is introduced to compensate for errors introduced by this assumption. Eq. (6.16) is Eq. (6.13) rewritten as a function of r_i , where s_i has been replaced by $\tilde{s}_i$ and a relaxation term $\beta \cdot (r_i - \tilde{r}_i)$ added to the exponent. It is easy to see that when the computed quantities approach the real ones, both methods recover the actual scatter-free scan given in Eq. (6.13). The advantage of Eq. (6.15) is that it is numerically stable, its disadvantage is a relatively slow convergence. The advantage of Eq. (6.16) is a very fast convergence, its main disadvantage is the fact that small errors in the scatter estimate lead to large errors in a_i in regions with large attenuation (*i.e.* large r_i) as seen from the following equation ($\beta = 1$ is used for the sake of simplicity):

$$\Delta a_i = \frac{x}{1-x} \frac{\Delta \tilde{S}_i}{\tilde{S}_i}, \quad x = \tilde{s}_i \exp(r_i) \quad (6.17)$$

and from the fact that x approaches unity for large r_i .

6.5 Benchmarking the scatter correction algorithm.

6.5.1 A water cylinder

As a first test for the proposed scatter correction algorithm, a simple homogeneous water cylinder (20 cm diameter $\times$ 20 cm length) is considered with the x-ray source rotating around the symmetry axis. Since the phantom is cylindrically symmetric, it is sufficient to compute the 0° projection only, obtaining all other projections by simply copying the 0° scan (128 projections are used in this example). In this first test the correction method given in Eq. (6.15) with $\alpha = 0$ is employed. Figure 6.5 (left

panel) shows a profile through the middle slice of the reconstructed attenuation image after the 0'th iteration (*i.e.* using the uncorrected scans r_i), 1'st and 5'th iterations. One can see how with each iteration step, the values of the attenuation coefficient approach the correct value of $\mu(60 \text{ keV}) = 0.21 \text{ cm}^{-1}$. The large fluctuations observed in the middle of the profile are due to the strong correlation when re-using the 0° projection for all 128 projections. The central points along the rotation axis are the most affected since exactly the same points are used in the reconstruction for this region. If one uses the LASG denoising algorithm to reduce the statistical noise, a much smoother profile is obtained and a faster convergence to the correct value of the attenuation coefficient is observed, as can be seen in the right panel of Fig. 6.5.

Figure 6.5: Profile across the middle slice of the reconstructed attenuation image of a water cylinder (10 cm radius, 20 cm length) for 128 projections. The scatter correction algorithm defined in Eq. (6.15) is used. The left panel shows the result without, the right panel with, denoising.

6.5.2 Water cube with 5 bone rods

A more challenging arrangement is a 30 cm^3 water cube with five bone inserts as shown on the left side of Fig. 6.9 (page 147). In this case the correction algorithm

Figure 6.6: Iterative correction shown for a profile across the middle slice ($64 \times 64 \times 64$, 0.5 cm voxels) for 60 keV x-ray beam on 30 cm^3 water phantom. Reconstruction done with 72 projections.

given in Eq. (6.15) with $\alpha = 0$ converges too slowly. Using $\alpha = 1$ initially improves the convergence rate, but after 6 iterations the change in each subsequent iteration is very small. Fig. 6.6 shows a comparison between the scatter-free scan (black line) and the estimated scatter-free scans after 0, 1 and 5 iterations along a line in the 0° scan. The measured scan (used to obtain the phantom in the 0'th iteration) is also shown with the blue line.

The influence of denoising is illustrated in Fig. 6.7, which shows the full-scatter scan (a), scatter-free scan (b), and reconstructed scatter-free scans after 5 iterations without (c) and with (d) denoising. The image in Fig. 6.7d is obtained with 10 times fewer particle histories compared to Fig. 6.7c, thus indicating that denoising brings at least another factor of 10 improvement in simulation speed.

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Figure 6.7: 0° scans of a water cube with 5 bone inserts with a 64×64 detector. (a) Initial uncorrected scan with full scatter. (b) Scatter-free scan obtained from direct simulation which is the goal of the scatter corrections. (c) Result of correcting the scatter without smoothing. (d) A smoothing procedure is used with 10 times less histories than when not smoothing.

6.5.3 Water sphere with spherical inserts of different composition

The FDK reconstruction algorithm employed in this study introduces significant artifacts near sharp edges. As a consequence, the actual phantom composition in these regions is not correctly reproduced. This in turn introduces errors in the es-

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Figure 6.8: The middle slice of the reconstructed attenuation image (left panel) and a profile through the center (right panel) of the phantom described in section 6.5.3.

estimated scatter distributions which are exponentially amplified in regions with significant attenuation according to equation 6.17. Therefore, a geometry with smooth boundaries, which is also more representative for practical applications than the water box with bone inserts from the previous section, is considered as a final example: a 15 cm radius water sphere with four spherical inserts of varying composition ($\rho = 1.1, 1.5, 1.6, 2.0 \text{ g/cm}^3$). The scatter correction algorithm defined in Eq. (6.16) with $\beta = 0.5$ is employed. However, it is found that the scatter distribution computed from a voxelized representation of the phantom must be corrected before use in Eq. (6.16). The correction is a simple shift determined from the requirement that the computed scan reproduces the measured scan in regions with no attenuation (*i.e.* regions that are not behind the scanned object) Figure 6.8 shows a profile across a central slice of the reconstructed sphere after the third iteration. In this case the algorithm converges faster and is also capable of faithfully reproducing the inserts of different density.

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6.6 Increasing scatter estimation efficiency

6.6.1 Calculation phantoms

The effect of different VRTs on the efficiency calculation of the scatter distribution is studied for two cases: a 16×16 pixels CBCT scan of a simple water phantom with bone inserts and a 256×256 pixels CBCT scan of a chest phantom taken from a voxelized human phantom. Both phantoms were irradiated with a 120 kV x-ray spectrum taken from a realistic BEAMnrc²⁹ simulation of a COMET MXR-320 x-ray tube. In both cases 360 projections at 1° intervals were computed. The first case is used for a rapid finding of how the calculation efficiency is affected by different VRTs. In the second case these VRTs undergo a more challenging test providing insight into how well these VRTs will perform on more realistic setups.

Figure 6.9: Phantoms used in this study. **Left:** Water phantom with 5 bone inserts. **Right:** Female Adult voXel (FAX06)¹⁸¹ chest phantom.

6.6.1.1 Water phantom with bone inserts.

The 120 kV x-ray beam was used to irradiate an XYZ geometry defining a $30 \times 30 \times 30 \text{ cm}^3$ water phantom comprised of 0.5 cm cubic voxels with 5 bone inserts (20 cm long, 2 cm wide and 2 cm high) as shown on the left side of Fig. 6.9. Bone composition was taken from the ICRU 44 report.¹⁸² The scoring plane was divided into 16×16 square pixels of 1.88 cm width.

Figure 6.10: Scatter efficiency as a function of detector resolution for an analog calculation (open circles) and a calculation using VRTs (solid circles) for the $30 \times 30 \times 30 \text{ cm}^3$ water phantom with bone inserts irradiated with a 120 kV x-ray beam. The ratio ϵ/A , where A is the pixel area, is shown to be constant for both cases (triangles).

The efficiency results obtained for this detector resolution are easily extrapolated to higher detector resolutions. Since $RMSE$ is inversely proportional to the square root of the pixel area, the efficiency is directly proportional to the pixel area or indirectly proportional to the number of pixels. This is demonstrated in Fig. 6.10 where the efficiency as a function of detector resolution is shown for an analog

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calculation and a calculation combining the VRTs from section 6.2 with PDIS.

Figure 6.11: Relative error distribution of the μ -values of the phantoms reconstructed from the scatter-free and the uncorrected scans of a FAX06 chest phantom. To obtain this distribution, a region by region comparison of the μ -values from the reconstructed phantoms (μ_{it}) with the actual μ -values (μ_0) is done.

6.6.1.2 Voxelized human chest phantom.

The Female Adult voXel phantom (FAX06)¹⁸¹ (see right side of Fig. 6.9) was irradiated with a 120 kV x-ray beam to produce a “measured” chest CBCT scan. The 0° projection corresponds with the beam incident on shoulder and arms (lateral projection) and the 90° projection corresponds with the beam incident on the chest (frontal projection). The “measured” scan was used to reconstruct a $30 \times 30 \times 30 \text{ cm}^3$ phantom of a human chest with 0.15 cm cubic voxels. The scoring plane is divided into 256×256 square pixels of 0.18 cm width. The phantom obtained from the uncorrected scan will be made out of materials with linear attenuation coefficients (μ -values) predominantly smaller than those of the actual phantom due to

the scatter contamination. This can be seen in Fig. 6.11 where the distribution of relative errors of the obtained μ -values compared with the actual μ -values are shown for phantoms reconstructed from the “measured” and the “scatter-free” scans. The phantom from the uncorrected scan shows a systematic bias of its μ -values indicating an underestimation of the actual phantom μ -values.

6.6.2 Efficiency gains in scatter estimation

Analog calculations are taken as the baseline for comparison with calculations progressively incorporating different VRTs. In this context, analog refers to scoring air-kerma without use of any of the VRTs described in section 6.2. On the left side of Fig. 6.12 the RMSE of the scatter signal from an analog calculation for the water phantom with bone inserts is shown to change periodically as a function of projection angle. The RMSE has a minimum at 0° , 90° , 180° and 270° and a maximum at 45° and its corresponding angles in the other 3 quadrants. This is probably due to the fact that when the beam is incident on one of the phantom faces the attenuation path of the photons reaching the detector is very similar while when the beam is incident along the diagonal the attenuation path varies from almost zero to the length of the diagonal. This increased variation of the attenuation of the photons reaching the detector causes the RMSE to be higher. As a consequence, the efficiency curve as a function of projection angle behaves exactly opposite to the RMSE curve as can be seen on the right side of Fig. 6.12.

A comparison of scatter efficiency curves for different combinations of VRTs is shown in Fig. 6.13 for the water phantom with bone inserts. *Forced detection* increases the efficiency by a factor of 3 over the analog calculation (open squares) as depicted by the open triangles. The mean free path transform (*MFPTR*) contributes an extra 24% efficiency increase (diamonds). Although not shown, the Woodcock tracing technique

Figure 6.12: Root mean square error of the scatter signal (left) and scatter calculation efficiency (right) as functions of the projection angle for an analog calculation for the water phantom with the bone inserts irradiated by a 120 kV x-ray beam.

increases the efficiency by 44 %. However, the largest gain in efficiency is obtained with the `splitting + RR` techniques. The FS approach increases the efficiency by about 52 times compared to the analog calculation (circles). The optimum splitting parameters N_p and N_s can be found through an efficiency study of these parameters. This could be as simple as running short calculations for a range of either N_p or N_s values while maintaining the other splitting number constant and finding those values that maximize the efficiency.

For the FS technique, $N_p = N_s = 70$ is found to maximize the efficiency of the scatter calculation. The efficiency increases 86 times with the RDIS technique compared to the analog calculation (solid squares). The optimal parameters for the RDIS technique are found to be $N_p = N_s = 120$, $N_{\min} = 40$, $N_{\max} = 1000$. The PDIS technique pushes the efficiency one order of magnitude higher (solid triangles). The optimum parameters found are $f_{\text{split}} \approx 0.8$, $N_s = 30$ for a maximum efficiency of 180 at 0° and a total efficiency gain of 360 times over the analog calculation.

The scatter efficiency as a function of projection angle for the chest phantom is shown in Fig. 6.14 for different `splitting + RR` techniques (open symbols).

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Figure 6.13: Efficiency curves comparison for the water phantom with the bone inserts irradiated by a 120 kV x-ray beam. *MFPTR* stands for mean free path transform.

Although not explicitly shown, *forced detection* and *MFPTR* are turned on. The efficiency in this case is more than 2 orders of magnitude smaller than in the water phantom case due to the much higher detector resolution used (256×256) and an increased number of geometrical regions ($200 \times 200 \times 200$). It is also interesting to notice that the efficiency curves here do not show the same periodic behavior as in the water phantom. When the rectangular beam is incident laterally at 0° , the fraction of the beam interacting with the phantom is minimal and thus the efficiency is the smallest. On the other hand, when the beam is incident frontally at 90° the beam coverage of the phantom is maximal and so the efficiency is the largest.

A comparison of all *splitting* + *RR* techniques for the chest phantom shows that *FS* improves the efficiency 25 times and *RDIS* 45 times. Optimum *splitting*

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Figure 6.14: Scatter efficiency curves for a chest phantom irradiated by a 120 kV x-ray beam when using different splitting + RR techniques (open symbols). Solid symbols represent a combination of VRTs with a 2D LAGS smoothing algorithm.

parameters were $N_p = 200$ and $N_s \geq 1000$ for FS and $N_p = 200$, $N_s \geq 1000$, $N_{\min} = 10$ and $N_{\max} \geq 1000$ for RDIS. The greater than or equal sign stands for negligible changes with increasing values of the parameter. A $20 \times 20 \times 20$ importance grid was used in these calculation. During this study little sensitivity of the efficiency with the grid size was observed. Of course, a very large grid size will compromise the efficiency due to larger differences between $\bar{K}_j$ and K_j^i . On the other hand, a too small grid size will also compromise the efficiency gains due to increased statistical fluctuations.

For PDIS however, the efficiency gain is not as large as before (only 58 times improvement) and is only marginally better than for the RDIS technique. The opti-

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mum splitting parameters found were $f_{\text{splt}} = 80$ and $N_s \geq 300$. A possible cause for this reduction in the efficiency gain is the fact that this time, a reconstructed phantom is used. The variations in the linear attenuation coefficient will make K_a^i differ much more from K^i . To counter this, an average attenuation coefficient μ was used as the attenuation medium to compute K_a^i instead of the most abundant medium in the phantom. This approach improved the efficiency slightly and the PDIS curve shown in Fig. 6.14 was obtained using it.

If the 2D LASG smoothing algorithm from section 6.2.4 is applied to the estimated scatter distribution, then the efficiency increases dramatically by over two orders of magnitude. This is shown in Fig. 6.14 by the solid symbols. The FS technique increases the efficiency by a factor of about 9.8×10^3 for the 0° projection compared to the analog calculation. RDIS and PDIS increase the efficiency by a factor of about 1.9×10^4 for the 0° projection. An attempt to further increase the efficiency, by extending the 2D smoothing algorithm to a 3D smoothing, showed no significant increase in the efficiency. A 3D smoothing algorithm uses not only the neighboring detector pixels from a given projection, but also pixels between neighboring projections.

6.7 Influence of photon scatter modeling on image reconstruction accuracy.

A possible way to further reduce simulation time could be by using simplified physical scatter models. However it is important that these simpler models do not introduce a systematic bias in the scatter distribution. The purpose of this section is to investigate the effect of the level of sophistication of photon interaction models on the computed scatter in CBCT and its influence on the accuracy of image reconstruction. If the

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simplest physical model of an independent atom with free electrons is able to provide a scatter distribution within a desired level of accuracy from the real distribution, then further gains in efficiency can be obtained by only modeling the Compton scattering according to the Klein-Nishina formula.¹⁸³ In contrast, if molecular interference effects in coherent scattering have a large impact on the scatter distribution, then the MC approach becomes unfeasible due to the lack of data for all relevant human tissues. Although one could resort to approximated models that use a set of basic data from which different human body tissues can be obtained through a weighted sum.^{184,185}

The focus of this study is Compton and coherent scattering. The influence of photo-absorption cross sections is of secondary importance because it only affects the amount of attenuation for the scattered radiation. As described in section 2.3.4, the treatment of the coherent process in EGSnrc is extended to allow the use of arbitrary photon coherent scatter form factors. In this study use is made of measured molecular form factors for coherent scattering taken from the paper by Peplow and Verghese⁹³ which are now distributed with EGSnrc. A 60 keV photon beam is used as representative of the 120 kV x-ray beam commonly used in CBCT. The average spectrum energy for a 120 kV tungsten x-ray beam from a COMET MXR-320 is about 68 keV and its effective energy 63 keV.

6.7.1 Photon scatter models.

Three photon scatter models are investigated:

- Compton interactions (incoherent scattering) are modeled according to the Klein-Nishina equation and there is no coherent scattering. This implies interactions with free electrons at rest and will be referred to in what follows as “simple”.

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- Compton interactions modeled in the relativistic impulse approximation (RIA) thus taking into account binding and Doppler broadening.⁹⁴ This is considered state-of-the-art for incoherent scattering. Coherent scattering is taken into account using independent atom approximation form factors (IAAFF). This model will be referred to as “RIA+IAAFF”.
- RIA incoherent scattering plus coherent scattering based on measured molecular coherent scattering form factors (MCSFF). This is the most accurate photon scatter model available and will be referred to as “RIA+MCSFF”.

“Measured” scans are computed using `egs_cbct` with the most realistic photon scatter models model, i.e., RIA+MCSFF. This eliminates the influence of detector response and permits the investigation of the influence of photon scatter modeling only. Images are reconstructed from the “measured” projections by means of the iterative procedure for scatter correction outlined in section 6.4 using the three photon interaction models described above to estimate the scatter.

6.7.2 Description of phantoms studied.

Several phantoms with different levels of sophistication are considered. First, a 30 cm diameter water sphere without and with spherical inserts will be considered. The spherical inserts are either four water spheres of 4 cm radius and varying density ($\rho = 1.1, 1.5, 1.6, 2.0 \text{ g/cm}^3$) or two 6 cm diameter inserts of adipose tissue ($\rho = 0.95 \text{ g/cm}^3$) and Kapton ($\rho = 1.42 \text{ g/cm}^3$). Taking advantage of the spherical symmetry the scans are only acquired for a 0° angle and then rotated 179 times in 1° intervals to obtain the desired number of 180 projections. The scanner resolution is 128×128 pixels of 1 cm^2 area. The initial study with the homogeneous water phantom is performed with a correction scheme that simply subtracted the scatter signal from the total signal. In

the case of the water phantom with different kinds of inserts, the correction algorithm is refined to take advantage of available information about the scatter signal in the “measured” scan. This is done by matching the computed scan with the “measured” scan in areas beyond the object’s shadow, where the signal is negative, i.e., where only scatter events are registered. In all three cases the FDK image reconstruction algorithm is used to produce a $128 \times 128 \times 128$ image.

In the second stage of this study, the more challenging case of a $200 \times 200 \times 200$ voxels human head phantom with 1.20 mm cubic voxels is chosen. The Female Adult voXel phantom (FAX06)¹⁸¹ is used as a virtual human from which CBCT scans could be taken. The number of projections are doubled in this case to 360 at 1° intervals and a scanner with a resolution of 512×512 square pixels of 0.78 mm width is modeled. The reconstructed image is obtained with the same dimensions as the original phantom using the OSEM iterative reconstruction algorithm.

Since one of the main goals of this study is to assess the relevance of including molecular interference effects in coherent scattering, one would want to be able to use molecular form factors with the FAX06 head phantom. However, no data is available for bone and soft tissue among the materials measured by Peplow and Verghese. To address this problem, two head phantoms were studied. The first one has its normal composition and no molecular effects are included in the simulation of the coherent scattering. This phantom is referred to as “head” and only simple and RIA+IAAFF scatter models are considered. A second head phantom is similarly constructed but bone is substituted with Kapton and soft tissue with human breast tissue. This phantom will be referred to as “fake head” and all three photon scatter models are considered. Although for the purpose of this work it would suffice to show the results for only the “fake head” phantom, results for both head phantoms are presented since the image segmentation algorithm to create density-based ramp files was improved

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while processing the “fake head” phantom.

Figure 6.15: **Top:** Scatter signals produced by a 30 cm water sphere with different photon scatter models (left: simple, center: RIA+IAAFF, right: RIA+MCSFF) for a 0° scan. **Bottom:** Central scatter profile for the same scan.

6.7.3 Spherical phantoms.

As pointed out in section 6.7.2, several phantoms are used to test the effect of the three photon scatter models in the correction algorithm, which vary in complexity.

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Initially, a homogeneous water sphere without and with spherical inserts is used to produce a scan. Switching to a water sphere with four spherical water inserts of varying density isolates the effect of varying densities but constant MCSFF. Two spherical inserts of different composition (adipose tissue and Kapton) are used to assess the importance of the MCSFF in the correction algorithm.

The scatter signal produced by the three photon scatter models for the 0° scan of a homogeneous water sphere is shown in the upper panel of Fig. 6.15. The simple model (left) produces a relatively smooth distribution of the scatter signal on the detector, while the RIA+IAAFF (center) and RIA+MCSFF (right) show a bright ring marking the edge of the spherical phantom where photons undergoing coherent scattering (small angular deflections) can reach the detector with minimal or no attenuation. Inside the bright ring on the right panel (RIA+MCSFF) there is an inner dark ring indicating a decreased number of scattered photons in this region. A plot of the scatter distribution along a central line is shown in the lower panel of Fig. 6.15. The valley in the middle of the profile is caused by the larger photon attenuation. The simple model underestimates the scatter contribution compared to the more accurate models. Although it seems that an upward shift of the scatter profile produced by the simple model would match the more accurate estimates in the valley region corresponding to the phantom. The only difference between RIA+IAAFF and RIA+MCSFF is a lower peak for MCSFF near the phantom edge accompanied by a small dip which corresponds to the dark inner ring noted above. Both these features are due to the decreased forward coherent scattering when molecular interference effects are taken into account.

Fig. 6.16 shows in its left panel the scatter signal for a “measured” 0° scan (upper left corner) of a water sphere with inserts of adipose tissue and Kapton. Also shown are the scatter signals for the same scan obtained from the reconstructed

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phantoms using the three photon scatter models. One can see that now, the inner dark ring has disappeared from the RIA+MCSFF scatter signal (upper right). The RIA+IAAFF scatter signal (lower left) looks similar to the RIA+MCSFF and again the simple model (lower right) has a smoothly distributed scatter signal. The right panel of this figure shows a comparison of the central scatter profile of the “measured” scan with those obtained using the estimated phantoms with the different scatter models. The disappearance of the small dip at the peak in the RIA+MCSFF scatter distribution indicates that the modest influence of MCSFF is below the detection limit of the FDK algorithm employed in the image reconstruction process. Despite the fact that the scatter distribution obtained with the simple model shows large differences with the rest, these differences are mainly located near the phantom edge and beyond.

Figure 6.16: **Left:** Scatter signals for a 0° scan of a 30 cm water sphere with 6 cm diameter adipose tissue and Kapton inserts. “Measured” (top left), RIA+MCSFF (top right), RIA+IAAFF (bottom left), simple (bottom right). **Right:** Central scatter profile for the same scan.

If the correction algorithm is working correctly, the estimated phantom should converge to the real phantom. Therefore, a practical way to quantitatively estimate

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the accuracy of the correction algorithm is to compare the “measured” scan with the scan obtained from the estimated phantom. This test could be used to establish the convergence criterion of the correction algorithm. Fig. 6.17 shows the relative RMSE of the scans obtained with the estimated phantoms for the three spherical phantoms included in this investigation as a function of the iteration number. In the case of the homogeneous water sphere (left panel), one can see that both, the simple and the RIA+MCSFF photon scatter models reproduce the measured scan with the same accuracy. However, for the water spheres with spherical inserts, both models that include coherent scattering and binding effects for Compton scattering, reproduce the “measured” scan with the same level of accuracy, while the simple model is noticeably less accurate.

Figure 6.17: Relative RMSE between “measured” scan of the real phantom and scans of the phantoms obtained using the MC scatter-corrected phantoms with different photon scatter models. **Left:** Homogeneous water sphere. **Center:** Water sphere with 4 spherical water inserts of varying density. **Right:** Water sphere with spherical adipose tissue and Kapton inserts.

The accuracy of the FDK reconstruction algorithm for a homogeneous water sphere with 180 projections and a $128 \times 128 \times 128$ voxels phantom is found to be about 3 % (MAPE). To remove this uncertainty from the comparison, and isolate the differences only due to the scatter correction algorithm, one can compare the estimated phantom with the phantom obtained from the scatter-free scan. Using the MRE in terms of the phantoms’ ρ values, one can follow the trend of the correction

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algorithm until it converges. Fig. 6.18 plots the MRE as a function of the iteration number for the three spherical phantoms. The left panel shows how both the simple and the RIA+MCSFF models produce phantoms that converge to the real homogeneous phantom with the same accuracy level. Once spherical inserts of different density are introduced (central panel), the simple model seems to underestimate the actual ρ values by 0.5 % while the RIA+IAA and RIA+MCSFF underestimate the real phantom in the first iteration but overestimate it by about 0.3 % and 0.2% after several iterations respectively. In the case of inserts of different composition (adipose tissue and Kapton) shown on the right panel, all three models overestimate the real phantom in the first iteration, but the simple model estimate decreases with the number of iterations converging to about a value of -0.5 %. The models including coherent scattering and Compton binding effects, converge to 0.2 % and 0.1% for RIA+IAAFF and RIA+MCSFF respectively.

It is also worth noticing that convergence in the homogeneous sphere case of Fig. 6.18 is much slower than the other two cases and that there are large fluctuations around the 0 % line. This is caused by the fact that the scatter correction algorithm did not include a shift based on a comparison of the “measured” scan and the scan at a given iteration step beyond the object’s shadow at the time when this phantom was analyzed.

That indeed there is convergence to the correct phantom in the homogeneous water sphere using both the simple and the most accurate model can be seen from the relative error distribution for the second and seventh iteration as shown in Fig. 6.19. At the second iteration step, the distribution is still asymmetrical showing a very large spread with a large negative mean value. By the seventh iteration, the error distribution has moved towards lower values tending to a more symmetrical shape and the spread in the errors is much less. From this figure one can also see that

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Figure 6.18: MRE between MC scatter-corrected phantoms with different photon scatter models and the phantom obtained from reconstructing a scatter-free scan. **Left:** Homogeneous water sphere. **Center:** Water sphere with 4 spherical water inserts of varying density. **Right:** Water sphere with spherical adipose tissue and Kapton inserts.

the spread and shape of the error distribution is not only influenced by the statistical noise, but also by the scatter correction and reconstruction algorithm. By the seventh iteration, the correction algorithm has converged and the Gaussian-like shape of the error distribution indicates that most of the errors left are statistical noise.

6.7.4 Head phantoms.

After testing the scatter models on simple spherical phantoms, the more challenging case of a human head phantom is studied. Although there is not a lot of scatter coming from a head phantom compared to a thorax or pelvis phantom, it is enough to introduce a significant bias in the reconstructed image. This is shown in Fig. 6.20 where a sagittal view of the 0° scan of a head phantom is shown with (center) and without (left) the contribution from the scatter. On the right, the distribution of errors relative to the actual phantom for both cases shows that the scatter is responsible for a 7.5 % bias.

A “measured” head phantom scan is obtained using the RIA+IAAFF photon scatter model since there is no measured data for the molecular form factors of bone and soft tissue. The “measured” scan is corrected for scattering to produce μ -based

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Figure 6.19: Relative error distributions for the second and the seventh iteration of the scatter correction algorithm for a spherical water phantom. Relative error shown is the relative density difference between the scatter-free FDK reconstructed phantom and the MC scatter-corrected phantoms. No shift of the scatter distribution was done to match the measured scan outside the object's shadow.

phantoms using the simple and RIA+IAAFF models. These MC scatter-corrected phantoms are compared in Fig. 6.21 to the real phantom using the relative RMSE as a measure of the error (squares). Four iteration steps of the correction algorithm are shown, clearly indicating convergence of the algorithm after the second iteration. The difference in the relative RMSE between the simple model (solid squares) and the RIA+IAAFF model (open squares) is only 0.2 %. The triangles in Fig. 6.21 show a similar comparison for the “fake head” phantom. In this case, RIA+MCSFF can be used since bone has been substituted with Kapton and soft tissue with human breast tissue. As in the head phantom, similar small differences are observed between

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Figure 6.20: Sagittal view of FAX06 head phantom (0° scan). Scatter free scan is shown on the left and the “measured” scan on the center. On the right, the distributions of relative errors when comparing the reconstructed phantoms using both scans with the real phantom are shown. If no scatter correction is done, a 7.5% bias is introduced in the reconstructed image.

the simple and the other two photon scatter models. Although the smallest relative RMSE for RIA+IAAFF and RIA+MCSFF is obtained after the first iteration where the difference with the simple model is 0.9 %. After the first iteration, the statistical noise seems to adversely affect the correction algorithm increasing the relative RMSE. The smaller values of the relative RMSE for the “fake head” case are explained by the fact that a better image segmentation technique was used when creating the ramp files after the phantom reconstruction at each iteration step.

The small difference observed above in the relative RMSE suggests that there is no significant gain in using a more complex photon scatter model to perform the scatter corrections. However, a different picture emerges if one plots the MRE as a function of the iteration steps as shown in Fig. 6.22 for both the head (left) and the “fake head” (right) phantoms. In this case the differences between the simple model and the RIA+IAAFF and RIA+MCSFF models are much larger than when using the relative RMSE. For the head phantom case, the simple model underestimates the real phantom by 1.7 % while as the RIA+IAAFF model underestimates the real phantom with a MRE of 0.2 %. The MRE for the “fake head” case with the simple model shows an underestimation of the real phantom of 1.5 %. Both models, the

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Figure 6.21: Comparison between MC scatter-corrected phantoms with different photon scatter models and the original phantom. Squares represent the results for a head phantom. Triangles show the results for a head phantom with bone replaced with Kapton and soft tissue by breast tissue (fake head).

RIA+MCSFF and the RIA+IAAFF overestimate the actual phantom by less than 0.3 %.

The observed RMSE and MRE differences can be explained from Eq. (6.12). If the RMSE and MRE values for the first iteration step of the head phantom are used to calculate σ , a value of 6.90 % for both the simple and the RIA+IAAFF models is obtained which dominates the value of the RMSE. Similarly in the “fake head” phantom case, the obtained σ values of 2.63 %, 2.49 and 2.48 % for the simple, RIA+IAAFF, and RIA+MCSFF models respectively, account for the RMSE differences observed. The spread of the errors in the “fake head” phantom is less than in the head phantom which is a result of the better image segmentation algorithm used

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Figure 6.22: Relative error between MC scatter-corrected phantoms with different photon scatter models and the original phantom. **Left:**FAX06 head. **Right:**FAX06 head. Bone substituted with Kapton and soft tissue by breast tissue (fake head).

during the processing of the “fake head” phantom.

If one looks at the distribution of the relative errors as shown in Fig. 6.23 for the first iteration step, one can see that the values of the error distribution are symmetrically spread around its mean value, the MRE. There is clearly a larger bias introduced by the use of the simple model compared to the more accurate models as already hinted by the MRE results. Moreover, the standard deviation σ of the distributions for the same phantom seem to be very similar in agreement with the results from Eq. (6.12).

Figure 6.23: Relative error distributions after the first iteration for the head phantom (**left**) and the “fake head” phantom (**right**). Relative error shown here is the relative difference between the μ values of the MC scatter-corrected phantom and the original phantom.

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Chapter 7

Conclusions

The main goal of this work is the development and implementation of new techniques and algorithms for the efficient simulation of x-ray beam systems and their transport through collimation systems, measuring devices and voxelized phantoms.

Significant improvements in the modeling of x-ray systems are obtained in Chapter 3. Extending the directional bremsstrahlung splitting (DBS) technique down to kilovoltage energies showed that the efficiency gains at these energies are even more significant than in the megavoltage energy range. The inefficiency of the bremsstrahlung production at these energies, especially for “narrow beam” geometries is successfully compensated, thus allowing x-ray tube simulations to become more practical. In subsequent chapters, challenging situations are tackled in which standard analog simulation of the radiation transport would have been impracticable even with the steady increase of affordable computing resources.

Accurate knowledge of the FAC correction factors are crucial for a primary standards lab where the the air-kerma and the exposure should be known to better than 0.5% one sigma uncertainty. The effects being corrected for are in many cases

so small, that long calculation times are required for accurate estimation of these corrections if no special techniques are applied. The possibility to accurately calculate these FAC corrections and the HVL offers the flexibility to compute these quantities for any beam quality in a reasonable amount of time without having to resort to lengthy and cumbersome measurements, which can be left for invaluable experimental verification.

New VRTs were implemented for the fast and efficient estimation of the scatter contribution to CBCT scans. This scatter estimation algorithm can be easily incorporated into any CBCT image reconstruction algorithm when accurate image reconstruction is required as in dose verification during RT.

The following sections present specific concluding remarks for chapters 3, 4, 5, and 6.

7.1 Efficiency study conclusions

A dramatic increase of calculation efficiency using the DBS technique of up to 6 orders of magnitude larger than the efficiency of simulations without splitting is observed. When using optimum splitting numbers for both techniques, DBS is shown to be 60 times more efficient compared to UBS, the only technique previously available for x-ray tube simulations and employed in previous EGS or BEAM studies. Compared to UBS simulations with the splitting number of 100 recommended for linac simulations, DBS is 2800 times more efficient. The large improvement in efficiency is very useful and permits the calculation of quantities such as fluence, kerma, and photon spectra, to a very low statistical uncertainty within a reasonable amount of computing time.

The theoretical derivation of efficiency as a function of splitting number presented in Kawrakow¹²⁰ is confirmed for the case of kilovoltage x-ray simulations. The

theory can therefore be employed to quickly determine the optimum splitting number for any given simulation before undertaking longer production runs. Given the strong dependence of the optimum splitting number on geometry details, incident energy, and scoring area, the approach discussed in Chapter 3 is very useful in practice.

7.2 FAC conclusions

A self-consistent set of correction factors is presented and its implementation in the new EGSnrc C++ user-code `egs_fac` is described. Correction factors are computed using full simulations of the x-ray tube and a detailed model of the FAC.

Excellent agreement with measured A_{att} , A_{scat} and A_{eloss} values is observed in the medium x-ray energy range. The newly introduced correction factors for backscatter (A_{b}), beam geometry (A_{g}) and lack of charged particle equilibrium along the beam axis (A_{cpe}) are negligible (A_{b} and A_{g}) or very small (A_{cpe} , which reaches 1.00015 at 250 kV). It is shown that the evacuated-tube technique used at NRC to measure the attenuation correction overestimates A_{att} by about 0.03% in this energy range. The observation that aperture leakage must be taken into account, noted in previous work,^{124,129,130} is confirmed by this investigation. The computed aperture correction for the MEES varies between 1.00055 and 1.0013 for the beam qualities investigated. Changes in the total correction A_{total} at these energies due to the inclusion of the aperture correction A_{ap} will still lie within the one sigma uncertainties (type A and B) assigned previously to these corrections.

In the low-energy range, the agreement of the scatter correction, A_{scat} , and the electron loss correction, A_{eloss} for both sets of beam qualities, between the MC calculations and values derived from previous measurements for a finite number of beam qualities can be considered good within the previously assigned one sigma

uncertainty of 0.2% and 0.1% respectively. These assigned systematic uncertainties are very conservative and rather arbitrary. One would need to validate the MC values against the original experimental values from Ritz¹²³ and assess whether the current practice of interpolating and extrapolating these corrections for arbitrary beam qualities is accurate. This approach has been used in many NMIs based on the fact that these corrections vary very slowly with beam quality. Nonetheless, our MC calculated values in the low energy region are systematically higher than these derived values although still within the stated one sigma uncertainties.

Large discrepancies found between MC calculated and measured $A_{\text{att,exp}}$ values can be explained with a scaling of the tungsten L-shell EII cross-sections by a factor of 1.8. The correction to account for the inconsistency of the evacuated tube technique, A_x and the newly introduced correction for backscatter, A_b , are non-negligible at low-energies and their combined effect will decrease the value of the total correction A_{total} by about 0.6% for the lightly filtered beams and 0.4% for the mammography beams. Ideally, a consistent set of corrections should be used. For instance, MC calculated corrections validated against experimental measurements. However, a detailed analysis of the impact of the uncertainties in the underlying photon and electron interaction cross sections must be performed before the methodology presented in this work can become the basis for correction factors used in the NRC primary standards for x-ray beams.

7.3 HVL conclusions

Physical processes relevant to low-energy photon interactions, as well as the most accurate cross sections must be included in the MC simulation to avoid significant errors in HVL calculations, which can be for instance as large as 6% when Rayleigh

scattering is not included in the medium energy range. Although the combined effect of omitting all these processes and using the older data seems to mitigate this difference, it can still be as large as 3.5%.

HVL values are sensitive to the definition of the interpolation grid of the photon cross sections. Although the best choice within the EGSnrc implementation, is to set the energy limits as tight as possible in the cross section table, the best approach would be to use a piecewise interpolation algorithm between the atomic absorption edges.

The 1% underestimation of the experimental HVL at 120 kV worsens with increasing tube potential, reaching 2.5% at a tube potential of 300 kV. This hardening of the spectrum in the medium energy range indicate the MC simulations are producing softer spectra. These discrepancies between calculations and measurements can be explained by either a 2% reduction of the photo-absorption cross section, or by slightly hardening the bremsstrahlung spectrum. Both required changes are within the reported uncertainties of the respective cross sections.^{77,116,117,155}

If a tungsten L-shell EII cross-sections scaling of 1.8 for the lightly filtered low-energy beams is accepted, the 5% to 8% overestimation of the experimental HVL points to increasingly harder spectra for the lightly filtered beams. The increasing trend of the disagreement with tube potential can be explained by the need to use more and more absorber material with increasing energy for the determination of the HVL. In this case, the photon cross section uncertainties would have an additive effect on the attenuation. No sensitivity to scaling of the tungsten L-shell EII cross-sections is seen in the HVL and A_{att} at 10 kV. This could be explained if the discrepancies observed at this energy are purely due to the uncertainty in the photon cross-sections.

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7.4 CBCT conclusions

A new EGSnrc code named `egs_cbct` for performing CBCT scatter computations is developed. Significant gains in the scatter calculation efficiency are achieved by combining several VRTs. The largest impact on the efficiency comes from the `splitting` + `RR` techniques. It was found that PDIS and RDIS outperform FS by a large margin. The superiority of PDIS over RDIS in the water phantom with bone inserts is most probably connected with the fact that the scoring contribution from each particle is nearly constant given that K_a^i is much closer to the actual scoring signal K^i than $\bar{K}_j$ could be to K_j^i since it is an average over a finite volume and also because the phantom is mostly water. This superiority of PDIS over RDIS is lost when applying them to a realistic phantom. Both techniques seem to perform equally well in this case. However, RDIS requires the optimization of a larger number of parameters, while PDIS seems conceptually simpler with only two parameters to be optimized. If the 2D LASG smoothing algorithm is combined with the splitting technique, then the efficiency increases dramatically by over two orders of magnitude.

To put the efficiency gain results into perspective, a simulation with a 3 % statistical uncertainty of the scatter signal for the phantom studied here would take approximately 4 days for one projection with an analog calculation and only 18 s using the best combination of the the VRTs investigated here with a 2D LASG smoothing algorithm. On the other hand, this huge efficiency increase is still far from allowing the use of this technique for real-time scatter corrections. If for instance, one would use a 512×512 detector of the same total area, the efficiency would decrease proportionally to the pixel area as shown in Fig. 6.10 and a 3 % uncertainty calculation would require about 72 s per projection using all VRTs. However, if a 10 % statistical uncertainty in the scatter were enough to reconstruct the phantom, the calculation would take 6.5 s per projection, which is already in the proximity of being of practical use if a

medium size computer cluster is available.

The proposed approach to correct CBCT images for scatter using only the results of a Monte Carlo simulation is shown to correctly reproduce the attenuation coefficients. Due to the limitations of the FDK reconstruction algorithm, objects with round boundaries can be better reproduced than objects with sharp edges. The investigations presented show that using the signal beyond the objects dimensions as representative of the actual scatter to shift the computed scatter distribution, together with the correction method defined in Eq. (6.16) produces the best convergence and contrast.

There is a clear bias in the reconstructed image introduced by the use of the simple photon scatter model. In the simpler phantoms this bias is about 0.5 % and in the head phantom case it is about 1.5 %. For a phantom with significantly more scatter, such as the case of a pelvis, or a thorax phantom, this bias could be significantly higher.

The inclusion of molecular interference effects in coherent scattering has no significant effect in the image reconstruction process. Only near boundaries between low and high density regions would a small effect be expected. Therefore, the lack of data for molecular coherent scatter form factors will not be an obstacle in the implementation of accurate scatter correction algorithms.

Coherent scattering must be included in the MC simulation of photon scatter in CBCT imaging when accurate phantom reconstruction is required as in the case of dose reconstruction and image-guided radiation therapy. Despite its limitations, the simple model could be used for the purpose of patient setup, which currently is the primary use of CBCT imaging and where the requirements on the accuracy of the reconstructed image are not as stringent.

7.4. CBCT CONCLUSIONS

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