**Validation of a novel
general cavity theory formalism**

by

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Abstract

For many years cavity ionization chambers have been the preferred detectors for measuring absorbed dose from ionizing radiation. Cavity theory formalisms relate the detector signal to a dose in the surrounding medium. Common cavity theories are straightforward to calculate but make limiting assumptions about charged particle fluences in the chamber and the medium. The choices that make them accurate are conceptually ambiguous and unrelated to physics first principles. This prohibits their general application across a wide range of physical conditions.

A novel general cavity theory is introduced which addresses some of the previous limiting assumptions of existing formalisms by explicitly determining the perturbation of charged particles in the medium due to the chamber cavity. This cavity theory removes the ambiguity and derives from first principles at the expense of increased complexity. The formalism converges to the Spencer-Attix cavity theory in the limit of Bragg-Gray conditions and to the ratio of mass-energy absorption coefficients in the large cavity limit.

The EGSnrc Monte Carlo simulation software is used to determine the expected dose ratios from full chamber dose calculations and to generate the input quantities to the novel formalism with regard to the air kerma formalism under Fano conditions. For 1.25 MeV incident photons the formalism is within 0.1% of full chamber calculated dose ratios for materials with atomic numbers $4 \leq Z \leq 29$, between 0.2–0.7% at 300 keV, and between 0.8–5.3% at 50 keV. Formalism dose ratios calculated from cobalt-60, and 120 kVp x-ray, spectra showed similar agreement with full chamber calculated dose ratios as the mono-energetic cases.

This new cavity theory is shown to be five times more accurate, on average, than Spencer-Attix for cavity heights of 1.39 mm, and 2.3 times more accurate, on

average, for cavity heights of 0.15 mm in 24 comparisons. Over all materials and incident energies investigated the new cavity theory tracks the trend of dose ratios as cavity size changes from 0.1 mm to 10 mm in height. Restrictions imposed by previous cavity theories are removed by this novel formalism derivation and it shows promise as a confirmation of modern Monte Carlo dose calculation methods.

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Statement of originality

This thesis is a summary of the author's work during the course of his Ph.D. program at Carleton University in partnership with the Ottawa Hospital. It is based on the manuscripts listed below, which are either in preparation or under review. Most of the results have been presented at local conferences and as an oral presentation at the international American Association of Physicists in Medicine and Canadian Organization of Medical Physics (AAPM/COMP) joint conference in Kelowna, BC (2020).

Dr. Miller MacPherson and Dr. Daniel La Russa supervised the research and provided input at all stages of presentations and publications. The author of this thesis performed all of the computational work, and drafted and revised the manuscripts. A description of where the results of each manuscript can be found in the thesis are shown below.

Peer-reviewed papers

I. A new cavity theory formalism based on a virtual source of charged particles:

I. Derivation from radiation transport equations

- The original theoretical background for this research was developed by Dr. Iwan Kawrakow, and prepared for publication by myself with input from co-authors.
- The results of this paper appear in chapter [2](#) and are the foundation for the following chapters.
- Parts of this paper were presented at local conferences and as an oral presentation at the joint AAPM/COMP conference.

II. Monte Carlo calculations of ion chamber cavity doses for benchmarking cavity theory formalisms in photon beams

- The results of this paper appear in chapter 4 when preparing the baseline dose ratio library for validating novel cavity theories.
- Parts of this paper were presented at local conferences and as an oral presentation at the joint AAPM/COMP conference.

III. A new cavity theory formalism based on a virtual source of charged particles:

II. Investigation of accuracy

- The results of this paper appear in chapter 5 when discussing the accuracy of the novel cavity theory introduced in 2.
- Parts of this paper were presented at local conferences and as an oral presentation at the joint AAPM/COMP conference.

I certify that, to the best of my knowledge, the content of this thesis is my own work. This thesis has not been submitted for any degree or other purposes. I certify that the intellectual content of this thesis is the product of my own work and that all the assistance received in preparing this thesis and sources have been acknowledged.

Contents

Abstract	ii
Acknowledgements	iv
Statement of originality	v
List of tables	x
List of illustrations	xii
Glossary	xiii
1 Introduction	1
1.1 General introduction	1
1.2 Cavity theory	2
1.2.1 Large photon cavity theory	5
1.2.2 Bragg-Gray cavity theory	7
1.2.3 Spencer-Attix cavity theory	9
1.2.4 Burlin cavity theory	11
1.3 Review of recent related work	12
1.4 Overview of thesis, motivations, goals	16
2 Novel cavity theory formalism	19
2.1 Introduction to the novel cavity theory formalism	19
2.1.1 Air kerma formalism	23
2.2 The stopping power ratio as an effective source	25
2.3 Derivation of the effective source	27

2.3.1	The transport equations	28
2.3.2	The effective source	29
2.4	Expression for the stopping power ratio	34
2.5	Results	36
2.5.1	Small cavities and the convergence to the Spencer-Attix stopping-power ratio	36
2.5.2	Large cavity sizes and convergence to $\left(\frac{\bar{\mu}_{en}}{\rho}\right)_{wall}^{air}$	38
2.5.3	An analytical expression for the fluence correction factor, K_{fl}	38
2.6	Summary	39
2.6.1	Restrictions on ϵ	41
2.6.2	General application of a generalized stopping power ratio	42
3	The EGSnrc Monte Carlo code system	44
3.1	Introduction	44
3.1.1	Monte Carlo simulations of radiation transport	45
3.2	EGSnrc overview	47
3.2.1	Dosimetric quantities of interest	47
3.2.2	Physical processes simulated	49
3.2.3	Simulation parameters	49
4	Generation and validation of a library of calculated ion chamber doses for investigating cavity theories	51
4.1	Introduction	51
4.2	Materials and methods	53
4.2.1	Monte Carlo simulations	53
4.3	Results	58
4.3.1	Monte Carlo calculation of ion chamber response	58
4.3.2	Simple versus full transport parameters	61
4.3.3	Rayleigh scattering in cavity	69
4.4	Summary	71
4.4.1	Monte Carlo user-code and dose scoring comparison	71
4.4.2	The effect of transport parameter choice on ion chamber cavity dose	72

5	Investigating the accuracy of the novel cavity theory formalism	74
5.1	Introduction	74
5.2	Methods	76
5.2.1	Monte Carlo calculations	76
5.2.2	Formalism terms	76
5.2.3	Spencer-Attix cavity theory calculations	78
5.3	Results	78
5.3.1	Calculation of cavity theory formalism inputs	78
5.3.2	Dose ratios	86
5.4	Summary	104
6	Conclusions	108
6.1	Overview	108
6.2	Summary and conclusions	109
6.3	Future work	112
	References	122

List of Tables

3.1	EGSnrc codes used to investigate dosimetric quantities	48
4.1	Chamber wall thicknesses for full buildup of charged particles	54
4.2	Dose simulation transport parameters	57
5.1	Maximum percent difference in dose ratio between formalism and expected values	87
5.2	Mean percent difference in dose ratio between formalism and expected values	88
5.3	Accuracy of Spencer-Attix cavity theory compared to direct Monte Carlo calculated dose ratios	98
5.4	Accuracy of cavity theory compared to direct Monte Carlo calculated dose ratios by energy and material	99
5.5	Accuracy of formalism and Spencer-Attix cavity theory compared to direct Monte Carlo calculated dose ratios by energy	101
5.6	Accuracy of formalism and Spencer-Attix cavity theory compared to direct Monte Carlo calculated dose ratios by material	101

List of Figures

1.1	Kerma and dose in a region of interest	4
1.2	Collision kerma and dose with depth in a medium	6
4.1	Idealized pancake ion chamber for simulations	55
4.2	Dose ratios for 1.25 MeV incident photons in beryllium and graphite	59
4.3	Dose ratios for 1.25 MeV incident photons in aluminum and copper	60
4.4	Ratios of dose ratios comparing transport parameters for 1.25 MeV incident photons	62
4.5	Ratios of dose ratios comparing transport parameters for 0.3 MeV incident photons	63
4.6	Ratios of dose ratios comparing transport parameters for 0.05 MeV incident photons	64
4.7	Comparing the effect of simulating atomic relaxations for 0.05 MeV incident photons	66
4.8	Comparing the effect of simulating photoangular sampling for 0.05 MeV incident photons	67
4.9	Comparing the effect of simulating atomic relaxations for 0.3 MeV incident photons	68
4.10	Reyleigh scatter and the <i>Fano</i> simulation in the cavity user code	70
5.1	Charged particle dose spectra, 1.25 MeV, $\epsilon = 1$ keV	79
5.2	Charged particle dose spectra comparing graphite and copper	80
5.3	Initial charged particle spectra for a 1.25 MeV incident photon beam	81
5.4	Initial charged particle spectra for three incident photon energies in copper	82
5.5	Energy deposition spectra, $\chi(E)$	84

5.6	Fractional energy deposition spectra, $\chi(E) / E$	85
5.7	Comparison between formalism and direct Monte Carlo calculated dose ratios for a 1.25 MeV incident photon beam and $\epsilon = 1$ keV	89
5.8	Comparison between formalism and direct Monte Carlo calculated dose ratios for a ^{60}Co incident photon beam and $\epsilon = 1$ keV	90
5.9	Comparison between formalism and direct Monte Carlo calculated dose ratios for a 0.3 MeV incident photon beam and $\epsilon = 1$ keV	91
5.10	Comparison between formalism and direct Monte Carlo calculated dose ratios for a 0.05 MeV incident photon beam and $\epsilon = 1$ keV	92
5.11	Comparison between formalism and direct Monte Carlo calculated dose ratios for a 1.25 MeV incident photon beam incident on a copper walled chamber with $\epsilon = 1, 3$, and 10 keV	94
5.12	Comparison between formalism and direct Monte Carlo calculated dose ratios for a 1.25 MeV incident photon beam incident on an aluminum walled chamber with $\epsilon = 1, 3$, and 10 keV	95
5.13	Comparison between formalism and direct Monte Carlo calculated dose ratios for a 0.3 MeV incident photon beam incident on an aluminum walled chamber with $\epsilon = 1, 3$, and 10 keV	96
5.14	Comparison between formalism and Spencer-Attix and direct Monte Carlo calculated dose ratios for a 1.25 MeV incident photon beam incident on a copper walled chamber with $\epsilon = 1, 3$, and 10 keV	102
5.15	Comparison between formalism and Spencer-Attix and direct Monte Carlo calculated dose ratios for a 0.05 MeV incident photon beam and $\epsilon = 1$ keV	103

Glossary of Terms

Δ	A parameter in Spencer-Attix cavity theory denoting the threshold kinetic energy of charged particles below which residual kinetic energy can be consider to be deposited locally. It is used to define the set of restricted mass-collisional stopping powers used in the formalism, where collisional energy losses are assumed to be restricted to be below Δ .
D_{air}^{Fano}	The absorbed dose to an air-filled cavity of an ion chamber due to an external source of photons under ‘Fano conditions’, where attenuation and scatter of the external source is ignored.
ϵ	A parameter in the general cavity theory formalism introduced here denoting the threshold for the creation and tracking of charged particles.
$\frac{\mu_{tr}}{\rho}$	The mass-energy transfer coefficient (units of <i>frac</i> cm ² g) for ionizing photon beams. The product of $\frac{\mu_{tr}}{\rho}$ with the photon energy fluence Ψ yields the kinetic energy release per unit mass, or kerma.
$\frac{\mu_{en}}{\rho}$	The mass-energy absorption coefficient (units of <i>frac</i> cm ² g) for ionizing photon beams. The product of $\frac{\mu_{en}}{\rho}$ with the photon energy fluence Ψ yields the collision kerma.
$\frac{S(E)}{\rho}$	The unrestricted linear stopping power is the energy lost by particles per path length in a medium, $S(E) = -\frac{dE}{dx}$, divided by the density of the medium.
$\frac{L_{\Delta}(E)}{\rho}$	The restricted linear stopping power is the energy lost by particles per path length in a medium, $L(E) = -\frac{dE}{dx}$, divided by the density of the medium, restricted to energy losses below a threshold kinetic energy value Δ .
$\chi(E)$	The energy deposition function, which represents the mean expected energy deposited by an electron of energy E in a detector cavity when the electron is located somewhere within that cavity.
Ψ	The energy fluence describes the energy flow in a photon beam and is defined as the amount of energy dE crossing a unit area dA ($\Psi = \frac{dE}{dA}$) in $\frac{MeV}{cm^2}$
AE, UE, AP, UP	Kinetic energy limits for the calculation and creation of photon (AP,UP) and electron (AE,UE) cross-sections in the EGSnrc Monte Carlo codes.

Boltzmann transport equations	Equations which describe the transport of radiation through matter.
Cavity theory	A discipline which relates the absorbed radiation dose in the cavity volume of a detector, total energy absorbed divided by the mass of the cavity volume, to the absorbed dose that would exist in the surrounding medium in the absence of the cavity volume.
ECUT, PCUT	Low energy Monte Carlo cutoff values for the transport of charged particles (ECUT) and photons (PCUT).
Fluence	The number of particles incident on a volume divided by the cross-sectional area of the region, or the total number of particles per unit area with which a material is irradiated.
KERMA	An acronym for the Kinetic Energy Released per unit MAAss by a photon beam in a medium.
Z	The atomic number of an element that defines the number of protons in its nucleus.

Chapter 1

Introduction

1.1 General introduction

Cancer poses a large and growing impact on the Canadian population and health care system. Nearly half of all Canadians are expected to be diagnosed with some form of cancer in their lifetime.¹ Despite the decrease in age-standardized cancer mortality rates since 1988, the number of new cancer cases and deaths have been increasing due to population increase and ageing. Research into improving the detection and treatment of cancer remains a high priority.

Ionizing radiation therapy, mainly in the form of photon beams, is a major treatment avenue for many cancers with about 40–50% of cases receiving radiation as part of their treatment in North America.^{2,3} The success of radiation therapy depends strongly on the accurate delivery of absorbed dose to the patient, which is inferred from an ion chamber measurement under standard conditions. Absorbed dose is defined as the amount of energy deposited in a region of interest divided by the mass of the region and will be discussed further in section 1.2. Dosimetry protocols have been published by professional organizations that relate ion chamber signal to ab-

sorbed dose.⁴⁻⁷

The most direct measurement method of radiation dose is calorimetry. Calorimetry is the science of determining the change in energy of a system – a tank of water in radiation dosimetry – by measuring the heat deposited by a known incident beam and is the most accurate method to account for the energy absorbed in matter by ionizing radiation. Water calorimetry is performed in an extremely precise and controlled manner because the temperature increases caused by the incident radiation are minute.⁸ This precludes its use from hospitals and is therefore only used in standards labs. However, most clinical dosimeters in Canada can trace their calibration back to a water calorimetry standard.

Ion chambers are commonly used for clinical radiation dosimetry. They are constructed with a gas-filled cavity across which an electric potential is held. When the detector is placed in an ionizing radiation beam, the electric potential collects ionized charged particles in real time. The charge readout on the detector is proportional to the energy deposited by the ionizing radiation. Cavity theory is a discipline which relates the absorbed radiation dose in the cavity volume of a detector, total energy absorbed divided by the mass of the cavity volume, to the absorbed dose that would exist in the surrounding medium in the absence of the cavity volume – in the same region occupied by the cavity volume.

1.2 Cavity theory

An important quantity related to dose is called kerma, which stands for Kinetic Energy Relaxed per MAss. This is the energy transferred to charged particles by uncharged particles in a very small, point-like, mass (dm) of material. For a mono-

energetic incident beam the kerma, K , is defined as

$$K = \frac{d\bar{E}_{tr}}{dm} = \Psi \left(\frac{\mu_{tr}}{\rho} \right), \quad (1.1)$$

where $(\frac{d\bar{E}_{tr}}{dm})$ is the energy transferred to charged particles per mass, $(\frac{\mu_{tr}}{\rho})$ is the mass-energy transfer coefficient and Ψ is the energy fluence of incident uncharged particles.

The collision kerma, (K_c) , is defined as the energy transferred from photons to charged particles per unit mass at a point of interest, exclusive of radiative energy losses. The radiation yield, g , is the fraction of energy lost to these radiative processes. Then the collision kerma can be written as

$$K_c = K(1 - g) = \Psi \left(\frac{\mu_{tr}}{\rho} \right) (1 - g) = \Psi \left(\frac{\mu_{en}}{\rho} \right) = \frac{d\bar{E}_{en}}{dm}, \quad (1.2)$$

where $(\frac{\mu_{en}}{\rho})$ is the mass-energy absorption coefficient, and $(\frac{d\bar{E}_{en}}{dm})$ is the energy transferred to charged particles per mass that are ultimately absorbed via ionizational interactions. Under the assumption that the defined volume is small enough such that radiative-loss photons escape the region, K_c can represent the energy absorbed by the medium if the number and energy of charged particles entering the region is the same as those exiting it. Under these circumstances charged particle equilibrium (CPE)⁹ exists and the dose, D , is the same as the collision kerma in the region,

$$D \stackrel{\text{CPE}}{=} K_c. \quad (1.3)$$

If the details of the incident beam are known, the kerma is generally easy to calculate and is independent of the specifics of the region of interest. However, it is almost impossible to measure directly and not a fundamental quantity when concerning the

biological effects of ionizing radiation. In contrast, dose is the energy absorbed ‘down-stream’ by charged particles set in motion and depends heavily on the geometry of the region of interest as energy losses vary with size. Given a fixed geometry, the dose deposited in the region depends on the energy of the incident beam. Additionally, dose is difficult to calculate, but is measurable and the primary factor in determining the biological effects of ionizing radiation. Figure 1.1 shows a pictorial difference between kerma and dose.

Equations 1.2 and 1.3 are important in that they equate a measured quantity, D , with a calculable quantity, K_e . With these assumptions in mind the next section will develop a foundational cavity theory.

Figure 1.1: Region of interest depicting the difference between kerma and dose. An uncharged particle (incident from left, red) transfers energy to a charged particle (kerma)(blue), which in turn transfers kinetic energy to other entities before leaving the region of interest. The dose is represented by charged particle tracks which terminate inside the region (green).

1.2.1 Large photon cavity theory

Suppose a non-mono-energetic photon beam is incident on a medium and the dose to a region of interest inside the medium is desired. The photons may interact with the medium in a variety of ways, via the photoelectric process, Compton scattering, and pair/triplet production, imparting energy to charged particles until they leave the region of interest or lose all their energy. As in figure 1.2, the collision kerma is at a maximum near the surface of the medium and decreases with photon attenuation. The dose to medium increases with depth in the medium as an increasing number of charged particles are set in motion and begin to deposit energy. Full build-up of charged particles occurs when the dose equals K_c , after which both decrease with depth in the medium. If two conditions are met in the region of interest, this full build-up of charged particles and CPE, the dose to this region is the collision kerma and therefore

$$D_{\text{med}} \stackrel{\text{CPE}}{=} \int_0^{E_{\text{max},\gamma}} \Psi_{\text{med}}(E) \left(\frac{\mu_{\text{en}}(E)}{\rho} \right)_{\text{med}} dE, \quad (1.4)$$

where $\left(\frac{\mu_{\text{en}}(E)}{\rho} \right)_{\text{med}}$ is the energy-dependent mass-energy absorption coefficient for the medium (med), $\Psi_{\text{med}}(E)$ is the differential photon energy fluence in the medium with respect to energy, and $E_{\text{max},\gamma}$ is the maximum incident photon energy. The full build-up of charged particles set in motion is achieved when the photon beam has a sufficient depth in the medium.

Next, a cavity type detector, such as an ion chamber, is used to determine the dose in the region of interest. If the ranges of charged particles, set in motion through interactions with the incident photon beam, are small compared to the size of the detector cavity, then the analytical equation for dose to the cavity of the detector is

Figure 1.2: The relationship between collision kerma and absorbed dose as a function of depth in a medium irradiated with a photon beam.

$$D_{\text{cav}} \stackrel{\text{CPE}}{=} \int_0^{E_{\text{max},\gamma}} \Psi_{\text{cav}}(E) \left(\frac{\mu_{\text{en}}(E)}{\rho} \right)_{\text{cav}} dE. \quad (1.5)$$

The dominant contribution to dose comes from photon interactions giving charged particles energy in the cavity material. If the simplistic assumption stands that the photon energy fluence is equal in the medium and detector cavity, then from equations 1.4 and 1.5 a ratio of doses is constructed

$$\frac{D_{\text{med}}}{D_{\text{cav}}} \stackrel{\text{CPE}}{=} \left(\frac{\bar{\mu}_{\text{en}}}{\rho} \right)_{\text{cav}}^{\text{med}} = \frac{\int_0^{E_{\text{max},\gamma}} \Psi_{\text{med}}(E) \left(\frac{\mu_{\text{en}}(E)}{\rho} \right)_{\text{med}} dE}{\int_0^{E_{\text{max},\gamma}} \Psi_{\text{med}}(E) \left(\frac{\mu_{\text{en}}(E)}{\rho} \right)_{\text{cav}} dE}, \quad (1.6)$$

where $\left(\frac{\bar{\mu}_{\text{en}}}{\rho} \right)_{\text{cav}}^{\text{med}}$ is the spectrum-averaged ratio of mass-energy absorption coefficients in the medium and detector, respectively, and ' $E_{\text{max},\gamma}$ ' is the maximum incident

photon beam energy. In this way cavity theory is able to determine the dose to the medium by measuring the dose absorbed in the detector cavity as long as the assumptions are fulfilled. However, the assumptions made above are not realized in practice, and therefore equation 1.6 is only the starting point for an accurately constructed cavity theory.

1.2.2 Bragg-Gray cavity theory

In 1936 three scientists—Louis Harold Gray, William Henry Bragg, and William Lawrence Bragg—published the seminal work on today’s cavity theory.¹⁰ Considering a fluence of primary charged particles (those initially set in motion by photons) crossing a boundary between two media, medium and cavity, the Bragg-Gray (BG) cavity theory postulates that the fluence of these charged particles would be identical on each side (*i.e.* negligibly perturbed) and that secondary charged particles (those set in motion by collisions with primary charged particles) would be in equilibrium (the same number and energy of particles entering the region of interest as leaving it). The two conditions which must be met for this cavity theory to be accurate are:

- The dimensions of the cavity must be small with respect to the range of charged particles passing through so that the fluence in the medium is unperturbed by the cavity.
- The absorbed dose to the cavity must be deposited only by charged particles crossing it (*i.e.* photon interactions in the cavity contribute negligibly to the dose).

The dose to the medium in the absence of the cavity is

$$D_{\text{med}} \stackrel{\text{CPE}}{=} \int_0^{E_{\text{max}}} \Phi_{\text{med}}^{\text{BG}}(E) \left(\frac{S(E)}{\rho} \right)_{\text{med}} dE, \quad (1.7)$$

where $\Phi_{\text{med}}^{\text{BG}}(E)$ is the differential fluence of primary charged particles in the medium with energy E , $\left(\frac{S(E)}{\rho}\right)_{\text{med}}$ is the energy-dependent unrestricted mass collisional stopping power in the medium, and E_{max} is the maximum energy of charged particles. This Bragg-Gray charged particle fluence includes only primary electrons set in motion, which are assumed to be in equilibrium, as indicated by the $\stackrel{\text{CPE}}{=}$ in equation 1.7. Delta rays (δ), also called ‘knock-on’ electrons, are secondary charged particles set in motion by primary charged particles, rather than photons, and are also assumed to be in equilibrium and deposited locally in this scenario.

Like the ratio of doses presented in equation 1.6, and assuming that the fluences are equal in both media, the BG formulated ratio of doses is equated to

$$\frac{D_{\text{med}}^{\text{BG}}}{D_{\text{cav}}^{\text{BG}}} \stackrel{\text{CPE}}{=} \left(\frac{\bar{S}}{\rho}\right)_{\text{cav}}^{\text{med}} = \frac{\int_0^{E_{\text{max}}} \Phi_{\text{med}}^{\text{BG}}(E) \left(\frac{S(E)}{\rho}\right)_{\text{med}} dE}{\int_0^{E_{\text{max}}} \Phi_{\text{med}}^{\text{BG}}(E) \left(\frac{S(E)}{\rho}\right)_{\text{cav}} dE} \quad (1.8)$$

where $\left(\frac{\bar{S}}{\rho}\right)_{\text{cav}}^{\text{med}}$ is the spectrum averaged ratio of unrestricted mass collisional stopping powers in the medium and detector, respectively. This cavity theory is generally accurate when the energy of the majority of charged particles is high enough to cross the cavity. It follows that the detector signal would be proportional to the volume of the cavity. Studies have shown that this behavior is not realized with changes in cavity size and gas pressure, as ion chamber detector signals show a non-linear trend.^{11–15} Additionally, achieving charged particle equilibrium is not practical when detector cavity sizes are large, or comparably sized, in relation to the range of incident charged particles.¹⁶

1.2.3 Spencer-Attix cavity theory

Experimental results for ion chambers, notably those with high atomic number (Z) wall materials, disagreed with Bragg-Gray cavity theory. Practically speaking, for a ^{60}Co beam incident on a graphite ion chamber, >95% of the charged particle fluence (both primary and secondary) in the chamber have energies above 20 keV; more so for higher-Z wall materials. Some commonly used ion chambers have ~ 5 mm cavity radii, and a charged particle with an energy of 20 keV can escape this air cavity. The Bragg-Gray theory vs. experiment disagreement was attributed to the theory not accounting for the dose deposited by secondary charged particles. In 1955 Spencer and Attix developed a theory that incorporated the impact of secondary charged particles.^{17,18}

To account for the dose deposited by secondary charged particles set in motion, a new low-energy threshold was introduced, which is referred to as delta (Δ) in the material stopping powers. All charged particles, primary and secondary, with energies above the threshold were explicitly accounted for while those below were assumed to be deposited locally. This “restricted” stopping power is denoted as L . The Δ value represents the mean energy required for an electron to cross and escape the cavity and thus accounts for the observed variation in ionization density with cavity size. The mass-restricted stopping powers, restricted to collisional energy losses below the chosen Δ , $\left(\frac{L\Delta}{\rho}\right)$, are used in place of the unrestricted stopping powers used by the Bragg-Gray theory, $\left(\frac{S(E)}{\rho}\right)$. Further work was done by Nystrom and Nahum, adding an explicit track-end term, to account for energy deposited by charged particles as they reach the end of their track (*i.e.* their kinetic energy drops below Δ). This residual energy is considered to be deposited locally as these charged particles are considered separately in the Spencer-Attix charged particle fluence, Φ^{SA} .¹⁹ Analogous

to the Bragg-Gray equation 1.8, the Spencer-Attix equation is

$$\frac{D_{\text{med}}^{\text{SA}}}{D_{\text{cav}}^{\text{SA}}} \stackrel{\delta\text{-CPE}}{=} \left(\frac{\bar{L}_{\Delta}}{\rho} \right)_{\text{cav}}^{\text{med}} = \frac{\int_{\Delta}^{\text{E}_{\text{max}}} \Phi_{\text{med}}^{\text{SA}}(E) \left(\frac{L_{\Delta}(E)}{\rho} \right)_{\text{med}} dE + \Delta \Phi_{\text{med}}^{\text{SA}}(\Delta) \left(\frac{S(\Delta)}{\rho} \right)_{\text{med}}}{\int_{\Delta}^{\text{E}_{\text{max}}} \Phi_{\text{med}}^{\text{SA}}(E) \left(\frac{L_{\Delta}(E)}{\rho} \right)_{\text{cav}} dE + \Delta \Phi_{\text{med}}^{\text{SA}}(\Delta) \left(\frac{S(\Delta)}{\rho} \right)_{\text{cav}}} \quad (1.9)$$

where $\left(\frac{\bar{L}_{\Delta}}{\rho} \right)_{\text{cav}}^{\text{med}}$ is the spectrum-averaged ratio of restricted mass collisional stopping powers in the medium and detector, respectively, and is analogous to $\left(\frac{\bar{S}}{\rho} \right)_{\text{cav}}^{\text{med}}$ in equation 1.8; $\Phi_{\text{med}}^{\text{SA}}(E)$ incorporates all charged particles, both primary and secondary, with energies above Δ . The track end terms, $\Delta \Phi_{\text{med}}^{\text{SA}}(\Delta) \left(\frac{S(\Delta)}{\rho} \right)_{\text{med or cav}}$, account for all charged particles which slow down below the Δ threshold and deposit all of their energy locally.

This theory accurately follows the experimental trends mentioned previously in section 1.2.2 as long as the incident beam energy is high, detector materials are radiologically similar to air, and detectors with small sensitive volumes – relative to the range of electrons – are used.^{13,20–23} For this reason it was used clinically for many years because it was quite robust and accurate in the energy ranges and detector configurations of interest.^{13,20,21,24} However, there is no general method to determine the value of Δ for different detector materials or incident beam energies to ensure accuracy.^{25,26}

The most common method for determining Δ has been to calculate the mean chord length (L) of a spherical cavity as $L = 4V/S$, where V is the volume and S is the surface area of the cavity. This method for determining the chord length has been validated even if the dimensions of the cavity are not spherical (*e.g.* plane parallel cavity and thimble shaped ion chambers).^{27–30} It has been shown that the value of Δ , however, is related to the error on the Spencer-Attix solution to the Boltzmann transport equation rather than to the kinetic energy required by an electron to cross the cavity.²⁶ The

above restrictions on Spencer-Attix cavity theory ensure that it is only applied in situations where the charged particle fluence, Φ^{SA} , can be approximated as the same in both medium and detector.

1.2.4 Burlin cavity theory

Equations 1.8 and 1.9 introduced a ‘small’ cavity theory. They are labeled thus because they required that the cavity be small compared to the ranges of charged particles crossing it. It also assumes that the charged particle fluence is unperturbed by the cavity and that equilibrium exists. A ‘large’ cavity theory was introduced in equation 1.6 which had a large cavity size relative to the ranges of primary electrons, but small enough such that it did not disturb the photon fluence in the surrounding medium. In 1966 T.E. Burlin proposed an ‘intermediate’ cavity theory which described the situation when the ranges of electrons were comparable to the size of the cavity.^{24,31–33} This dose ratio is the weighted combination of ‘small’ and ‘large’ contributions and is written as

$$\frac{D_{\text{cav}}}{D_{\text{med}}} = d \left(\frac{\bar{L}_{\Delta}}{\rho} \right)_{\text{cav}}^{\text{med}} + (1 - d) \left(\frac{\bar{\mu}_{\text{en}}}{\rho} \right)_{\text{med}}^{\text{cav}}, \quad (1.10)$$

where $\mathbf{d}$ is a weighting parameter that varies between 0 and 1 as a function of cavity size, chamber material composition, incident photon energy, and at times, the cavity surroundings.

Like the Δ threshold, the $\mathbf{d}$ parameter does not have an accepted, *a priori*, method for determining its value.³⁴ Burlin himself used the equation $d = (1 - e^{-\beta L}) / (\beta L)$ where $L = 4V/S$ is the mean chord length of a spherical cavity and β represents the contribution to the cavity dose from charged particles originating in the medium and cavity. Further investigations have calculated $\mathbf{d}$ in a variety of ways with varying

degrees of success in various materials and incident energies.^{24,35-37} In the early 1980's a flurry of activity surrounded proposed modifications to Burlin's theory but their practical use is not clear.³⁸⁻⁴⁴ More recent work by Kumar *et al.* (2016) describe a computational approach to determine both Spencer-Attix's Δ and the $\mathbf{d}$ factor, but place a large computational overhead on the user.

1.3 Review of recent related work

The development of additional cavity theories has continued over the years.⁴⁵⁻⁵⁰ However, none of these have been put into routine use. Some of the theories made derivational assumptions and used approximations which limited their broad application, like Spencer-Attix cavity theory, while others have not been thoroughly investigated and their general applicability is therefore unknown. A possible reason for the lack of investigation is that Spencer-Attix cavity theory worked sufficiently well in the situations that were presented in the clinical radiation therapy energy regimes, when paired with radiologically similar graphite (or plastic) walled, air filled, ion chamber detectors, that there was no need for change. Additionally, Spencer-Attix is conceptually straightforward at the expense of a small trade-off in accuracy in most situations. However, as technology advanced the field – including a broader range of incident beam energies, smaller and non-standard radiation beam configurations, and an interest in alternative chamber materials – new approaches have become necessary.

In 2012 Bouchard published “A Theoretical Examination of Spencer-Attix Cavity Theory.”²⁶ The Boltzmann transport equations were used to comprehensively re-derive the generalized energy deposition of an Spencer-Attix-like model for all particle types, charged and uncharged. In special cases this theory was shown to mathematically reduce to the same dose relationships of the ‘small’ cavity theory in

section 1.2.3, and to the ‘large’ cavity theory in section 1.2.1. The accuracy of the formalism, however, remains to be thoroughly examined. Regardless, it showed that there are inconsistencies in the way the Spencer-Attix Δ cut-off energy is chosen to calculate dose ratios, and consequently the perturbation factors used to make this imperfect theory work for realistic detectors. He concluded that a new formalism of cavity theory suitable with the Monte Carlo (chapter 3) approach to detector response modelling would be preferable over attempting to refine the Spencer-Attix formalism with more correction factors.

In 2016 Kumar and Nahum explored the boundaries of Spencer-Attix cavity theory in “Dosimetric Response of Variable-Size Cavities in Photon-Irradiated Media and the Behaviour of the Spencer-Attix Cavity Integral with Increasing Δ .”²⁰ The authors reported ‘closely-equal’ agreement between Monte Carlo (section 3.1.1) calculated dose ratios and three cavity theories (‘large’ section 1.2.1, Spencer-Attix section 1.2.3, and Burlin section 1.2.4) in water, aluminum, and copper media irradiated by 1- and 10-MeV photon beams under quasi-charged particle equilibrium. A closer investigation of the Spencer-Attix cavity theory showed that it did not accurately predict dose ratios in various media when Δ was increased above 30 keV because there were too many secondary electrons with initial energies below this threshold. Therefore, an electron ‘detour factor’ (which took into account the changes in direction an electron undergoes when slowing down in matter due to elastic scattering, calculated by $DF = \frac{R_{csda}}{R_{50}}$) was investigated, requiring additional computation, which allowed the Spencer-Attix cavity theory to predict dose ratios within 2% of Monte Carlo calculated dose ratios in an air filled cavity surrounded by water for a wide range of incident photon beam energies. The electron ‘detour factor’ also allowed Spencer-Attix cavity theory to accurately predict dose ratios for a silicon medium in

water when the medium had an artificially imposed gas-like density. At higher silicon densities the ‘intermediate’ Burlin cavity theory (section 1.2.4) dose ratios showed ‘satisfactory’ agreement with Monte Carlo calculated dose ratios. When the new electron ‘detour factor’ was applied, the Spencer-Attix theory was able to accurately estimate the Burlin d parameter as a function of changing silicon density.

Their work also outlined a methodology for determining the maximum size of a cavity which exhibits Bragg-Gray qualities and provides guidance on the selection of Δ for high-energy photon beams to ensure an acceptable level of accuracy. Regarding Burlin cavity theory, this approach provided some guidance on how to determine the d parameter using Monte Carlo methods. Despite these results, the restrictions on Spencer-Attix cavity theory – only being valid for high incident energy photon beams and for radiologically similar materials – remain unchanged, and there is still no way to decide on the value of Δ to ensure an accurate prediction of dose ratios over a wider range of conditions. The paper used experiments requiring charged particle equilibrium and arbitrarily changing Δ values to obtain better agreement, both of which were shown previously to be of little value.^{25,51} Additionally, adding another correction factor, the electron ‘detour factor’, presented barriers to using cavity theory because it increased the complexity of calculation and may encourage users to find more practical avenues.

There is renewed interest in radiotherapy applications in the low photon energy range (kilovoltage) for small animal studies and kV breast and eye cancer therapy.^{52–56} Specifically, in 2017 Oliver and Thomson investigated “Cavity Theory Applications for Kilovoltage Cellular Dosimetry.”²⁴ This article reports a Monte Carlo investigation to compare the ‘large’, ‘small’ (Spencer-Attix), and ‘intermediate’ cavity theories (additionally comparing five different methods of determining the d parameter) to link

model-based dose calculation algorithms with energy deposition in cellular targets. The best overall agreement was found with the Burlin-Janssens approach³⁶ to calculating $\mathbf{d}$ and Spencer-Attix cavity theory was shown to perform poorly. Spencer-Attix cavity theory was not expected to produce the best results since the incident energies investigated were outside the recommended guidelines for accuracy. It was determined that using individualized approaches – applying the most accurate theory in a each of the ranges of situations tested and putting together a composite cavity theory – could lead to improved agreement, but such an approach would be prohibitively complex and be limited to specific situations. Additionally, further investigation would be required to establish a more general, universally-applicable, approach.

As computing power has dramatically increased in recent years the use of the Monte Carlo method became a viable alternative to, then began to replace, cavity theory for accurate calculations of cavity dose ratios.^{34,57–59} Direct calculations of dose ratios by Monte Carlo methods have formally replaced cavity theory in at least one metrology and standards setting.⁵

A more recent alternative to Monte Carlo that also takes advantage of increased computing power is the direct solution of the linear Boltzmann transport equations,^{60,61} which has more recently been applied to dose calculations in radiation therapy.^{62,63} The motion of individual charged particles, which deposit dose, can be described mathematically by these equations.^{64–66} Briefly, the transport equations describe the processes that radiation particles undergo as they pass through a medium. Considering a fluence of particles with direction at a point in space, the gradient of this fluence depends on the addition to, or loss from, this point due to scattering events. The change in fluence in one direction will affect the fluence in other directions so that energy conservation applies. For a given particle type the equation is

written

$$\vec{\Omega} \cdot \vec{\nabla} \Phi(E, \vec{\Omega}, \vec{x}) = \rho(\vec{x}) \left[S(E, \vec{\Omega}, \vec{x}) + I(E, \vec{\Omega}, \vec{x}) \right]. \quad (1.11)$$

Here, $\vec{x}$ and $\vec{\Omega}$ are the position and direction vectors, respectively, $\vec{\nabla}$ is the gradient operator, E is the energy (in MeV), $\Phi(E, \vec{\Omega}, \vec{x})$ is the particle fluence differential in energy and direction (in $\text{MeV}^{-1} \text{ cm}^{-2} \text{ sr}^{-1}$), and $\rho(\vec{x})$ is the mass density distribution (in m/cm^3). $S(E, \vec{\Omega}, \vec{x})$ and $I(E, \vec{\Omega}, \vec{x})$ are the source and interaction terms (in $\text{MeV}^{-1} \text{ cm}^{-2} \text{ sr}^{-1}$), representing the differential number of particles generated locally per unit mass by a source and from interactions, respectively. The source term is defined by the beam, and the interaction term is an operator on the fluence describing all physical interactions in the medium. For electrons it describes elastic scattering, inelastic scattering, bremsstrahlung production etc.⁵¹ In chapter 2 the main subject of this thesis, a novel cavity theory formalism, will be introduced and developed in relation to equation 1.11. Additional information can also be found in Bedford or Spencer.^{18,62}

1.4 Overview of thesis, motivations, goals

Despite the inability of cavity theories to predict dose ratios over a wide range of conditions, and the recent adoption of alternative methods for determining dose ratios, it is important to continue their development. Cavity theory is the only approach to understanding how detector measurements relate to dose and it is profitable to maintain our understanding of the link between these two fundamental quantities. The most popular historical formalisms have straightforward mathematical implementations, but rely on conceptually ambiguous arguments to chose parameters and ensure accurate results under narrowly defined conditions. In this work a new cavity the-

ory formalism is introduced using approaches similar to Bouchard²⁶ and Luo⁴⁷ that has the potential to be applicable over a broader range of situations than previous theories. This novel formalism will be developed from first principles and specifically address the ambiguous arguments made by previous cavity theories. This approach is more mathematically complex, but it is hypothesized to be more generally applicable, more accurate, and can be applied in a more consistent manner than the methods mentioned previously. These properties ensure its timely application over the broadest range of physical conditions.

Despite the increase in computing power mentioned in section 1.3, time is an important factor. The computing resources required for direct Monte Carlo methods of calculating ion chamber cavity doses are not widely available, and take orders of magnitude longer than corresponding cavity theory calculations. Consequently, there is the potential for this formalism to fill a valuable role as a user accessible confirmation tool that has its foundation in the physics of cavity theory.

Chapter 2 derives the formalism evaluated here from first principles, the linear Boltzmann transport equations, and discusses its relationship with known cavity theory foundations – reducing to Spencer-Attix cavity theory in the ‘small’ cavity sized limit (equation 1.9) and reducing to the ratio of mass energy absorption coefficients in the ‘large’ cavity size limit (equation 1.6). In particular, the perturbation of the charged particle fluence, by the cavity, is handled explicitly, and is at the heart of the differences in relation to prior theories. The restrictions on the proposed theory are also discussed.

Chapter 3 introduces the Monte Carlo software with its various relevant calculation parameters and describes the methods of calculating dose ratios used to evaluate the accuracy of ion chamber response in photon beams. Chapter 4 develops and calcu-

lates benchmark dose ratios using two **EGSnrc** Monte Carlo simulation codes. These dose ratios in various media and air create a library of values across a wide range of conditions and input parameters so that a thorough investigation of the novel cavity theory is possible. The parameters and pitfalls associated with accurate Monte Carlo calculations will be discussed. Chapter 5 covers the investigation into the accuracy of the novel formalism by comparing it against bench-marked Monte Carlo calculated values from chapter 4 and against Spencer-Attix theory calculated values. In chapter 6 the applicability of the cavity theory is summarized and its relevance to the field is discussed.

Chapter 2

Novel cavity theory formalism

2.1 Introduction to the novel cavity theory formalism

A brief introduction to cavity theory was given in section 1.2. Here we introduce an alternative formalism that is unconstrained by the ‘Bragg-Gray’ conditions laid out in section 1.2.2. The following will lay out the groundwork for deriving the necessary dose ratios, and is similar to the approach taken by Bielajew.⁶⁷ Consider the dose to an air cavity filled with dry air, D_{cav} , of a thick walled ion chamber, free in air, due to an uncontaminated broad parallel photon beam. This is written

$$D_{cav} = D_0 + D_s \tag{2.1}$$

where D_0 is the dose deposited by charged particles set in motion by the primary photon beam and D_s is the dose deposited by charged particles set in motion by scattered photons, bremsstrahlung radiation, positron annihilation, and fluorescent

x-rays. Multiplying and dividing by D_0 gives

$$D_{cav} = \frac{D_0 + D_s}{D_0} D_0 = A_{scatt} D_0, \quad (2.2)$$

where A_{scatt} is the ratio of total dose deposited in the cavity to the dose attributed solely to interactions of primary photons. Similarly, introducing the effect of photon attenuation,

$$D_{cav} = A_{scatt} \frac{D_0}{D_1} D_1 = A_{scatt} A_{att} D_1 = A_{wall} D_1, \quad (2.3)$$

where D_1 is the dose in the cavity, deposited by charged particles, due to a photon beam that is not attenuated, and A_{att} is the ratio of dose due to primary photon interactions to the dose due to an unattenuated photon beam (one where primary photons are “regenerated” after an interaction that results in energy loss and/or a change in direction). A_{wall} is the product of the two previous correction factors and is grouped thus because both originate predominantly in the chamber wall medium.

Now consider the dose to the air cavity under a special fluence,

$$D_{cav} = A_{wall} \frac{D_1}{D_2} D_2 = A_{wall} A_{fl} D_2, \quad (2.4)$$

where D_2 is the dose to the cavity due to the electron fluence resulting from an unattenuated, unscattered photon beam that one would observe at the position of the cavity without the cavity present (*i.e.* the dose due to a charged particle fluence in an infinite wall medium). A_{fl} is defined as the correction for the perturbation of the electron fluence due to the presence of the cavity. Introducing the dose to the

wall medium, D_{cav} is

$$D_{cav} \stackrel{\delta-CPE}{=} A_{wall} A_{fl} \frac{D_2}{D_3} D_3 = A_{wall} A_{fl} \left(\frac{\bar{L}_\Delta}{\rho} \right)_{wall}^{air} D_3, \quad (2.5)$$

where D_3 is the dose due to the unperturbed electron fluence (from an unattenuated, unscattered photon beam) at the position of the cavity with the cavity removed (*i.e.* dose to a uniform wall medium). Under these conditions, the ratio of $\frac{D_2}{D_3}$ is historically estimated by the Spencer-Attix ratio of collisional mass-restricted stopping powers from equation 1.9. From energy conservation and, by definition, under the conditions of charged particle equilibrium, D_3 is equal to the product of the photon energy fluence, Ψ_0 , and the spectrum-averaged mass-energy absorption coefficient, $\left(\frac{\bar{\mu}_{en}}{\rho} \right)_{wall}$ (also known as the collision kerma in the wall medium, $(K_c)_{wall}$, given by equation 1.2),

$$D_{cav} \stackrel{\delta-CPE}{=} A_{wall} A_{fl} \left(\frac{\bar{L}_\Delta}{\rho} \right)_{wall}^{air} \Psi_0 \left(\frac{\bar{\mu}_{en}}{\rho} \right)_{wall}. \quad (2.6)$$

Here it must be noted that both A_{fl} and $\left(\frac{\bar{L}_\Delta}{\rho} \right)_{wall}^{air}$ depend on the size of the cavity.^{25,68} It is expected that larger cavities will perturb the charged particle fluence more than smaller cavities, therefore A_{fl} will increase with cavity size. Likewise, the value of Δ in $\left(\frac{\bar{L}_\Delta}{\rho} \right)_{wall}^{air}$, denoting the mean energy of an electron needed to cross the cavity, and therefore $\left(\frac{\bar{L}_\Delta}{\rho} \right)_{wall}^{air}$, will also change with cavity size. Kawrakow suggested that A_{fl} be ignored and all fluence perturbations be accounted for in a new stopping power ratio since there was no good reason to have two ‘cavity-size dependent’ parameters.⁶⁸ Therefore, equation 2.6 is re-expressed as

$$D_{cav} = A_{wall} \frac{D_1}{D_3} \Psi_0 \left(\frac{\bar{\mu}_{en}}{\rho} \right)_{wall} = A_{wall} \left(\frac{\bar{L}_\epsilon}{\rho} \right)_{wall}^{air} \Psi_0 \left(\frac{\bar{\mu}_{en}}{\rho} \right)_{wall}, \quad (2.7)$$

2.1. INTRODUCTION TO THE NOVEL CAVITY THEORY FORMALISM

where $\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air} = A_{fl} \left(\frac{\bar{L}_\Delta}{\rho}\right)_{wall}^{air}$. The Greek letter epsilon, subscript ‘ ϵ ’, is chosen to distinguish this stopping power ratio from that of the Spencer-Attix formalism, which relies on Δ . This new formulation implicitly assumes charged particle equilibrium below an energy threshold ϵ , although it takes on a different meaning and has implications that are separate and distinct from the requirements in the Spencer-Attix formalism. Restrictions on the value of ϵ are presented in section 2.6.1. Rearranging equation 2.7 for the new stopping power ratio,

$$\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air} = \frac{D_{cav}}{A_{wall} \Psi_0 \left(\frac{\bar{\mu}_{en}}{\rho}\right)_{wall}}. \quad (2.8)$$

Dividing $(K_c)_{air} = \Psi_0 \left(\frac{\bar{\mu}_{en}}{\rho}\right)_{air}$ in the numerator and denominator,

$$\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air} = \frac{\frac{D_{cav}}{(K_c)_{air}}}{A_{wall} \left(\frac{\bar{\mu}_{en}}{\rho}\right)_{air}^{wall}} = \frac{K_{wall} D_{cav} \left(\frac{\bar{\mu}_{en}}{\rho}\right)_{wall}^{air}}{(K_c)_{air}}, \quad (2.9)$$

where $K_{wall} = \frac{1}{A_{wall}}$ and $\left(\frac{\bar{\mu}_{en}}{\rho}\right)_{wall}^{air}$ is the spectrum-averaged ratio of mass-energy absorption coefficients. Recalling the definition of D_{cav} in equation 2.7, the new stopping power ratio reduces to,

$$\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air} = \frac{D_1}{(K_c)_{wall}} = \frac{D_1}{D_3} \equiv \frac{D_{air}^{Fano}}{D_{wall}^{Fano}}, \quad (2.10)$$

where D_{air}^{Fano} is the dose to the air cavity deposited by charged particles set in motion by an unscattered, unattenuated, broad-parallel photon beam, and D_{wall}^{Fano} is the collision kerma in the same wall medium from the same incident photon beam. The ‘Fano’ superscript refers to the specific conditions described above, namely the absence of

attenuation and scatter, which were among the conditions imposed by Ugo Fano in his 1954 paper.⁶⁹

2.1.1 Air kerma formalism

As an initial, practical application of this new formalism, we turn to the problem of determining air kerma for an external photon source. Specifically, and for the sake of those unfamiliar with the field, we refer to the determination of using an ion chamber free-in-air, and where the effects of attenuation, scatter, and point like nature of the source of photons are treated separately with correction factors.

For a fully corrected charge (of one sign), Q_{air} , liberated in the air-filled cavity of an ion chamber by an external source of photons, the air kerma, K_{air} is given as

$$K_{air} = D_{air} \left(\frac{\bar{L}_{\Delta}}{\rho} \right)_{air}^{wall} \left(\frac{\bar{\mu}_{en}}{\rho} \right)_{wall}^{air} \frac{1}{(1 - \bar{g}_{air})} K_h K_{wall} K_{an} K_{comp} K. \quad (2.11)$$

Substituting for D_{air} results in the traditional form of the air kerma equation

$$K_{air} = \frac{Q_{air}}{m_{air}} \left(\frac{W}{e} \right)_{air} \left(\frac{\bar{L}_{\Delta}}{\rho} \right)_{air}^{wall} \left(\frac{\bar{\mu}_{en}}{\rho} \right)_{wall}^{air} \frac{1}{(1 - \bar{g}_{air})} K_h K_{wall} K_{an} K_{comp} K. \quad (2.12)$$

In equation 2.12 the charge Q_{air} collected is often corrected for ion recombination and polarity effects due to the electric potential applied between the ion chamber anodes. When using vented ion chambers, the standard temperature-pressure correction is used to correct for the effects that deviations in temperature and pressure, from reference conditions, have on the mass of air (m_{air}) filling the cavity volume. The quantity $\left(\frac{W}{e} \right)_{air}$ is the mean energy deposited in air per unit charge of one sign released, and $\bar{g}_{air}$ is the mean fraction of energy lost to radiative processes. The effects of humidity, attenuation and scatter, beam anisotropy, wall heterogeneities, and var-

2.1. INTRODUCTION TO THE NOVEL CAVITY THEORY FORMALISM

ious other non-ideal conditions (e.g. stem effects, radial non-uniformity of the beam, etc) are corrected for by the factors K_h , K_{wall} , K_{an} , and K , respectively, and formally defined elsewhere.^{70–72} With these correction factors included in the formalism, the Spencer-Attix wall-to-air stopping-power ratio $\left(\frac{\bar{L}_\Delta}{\rho}\right)_{air}^{wall}$ in equation 2.12 represents the ratio of the dose to the air in the cavity to the dose in the wall medium due to an unattenuated, unscattered, broad-parallel photon beam. Similar to equation 1.9, $\left(\frac{\bar{L}_\Delta}{\rho}\right)_{air}^{wall}$ is expressed as

$$\left(\frac{\bar{L}_\Delta}{\rho}\right)_{air}^{wall} \stackrel{\delta-CPE}{=} \frac{D_{wall}^{Fano}}{D_{air}^{Fano}} \approx \frac{\int_{\Delta}^{E_0} dE \Phi_{wall}(E) \left(\frac{L_\Delta(E)}{\rho}\right)_{wall} + \Delta \Phi_{wall}(\Delta) \left(\frac{L_\Delta(\Delta)}{\rho}\right)_{wall}}{\int_{\Delta}^{E_0} dE \Phi_{wall}(E) \left(\frac{L_\Delta(E)}{\rho}\right)_{air} + \Delta \Phi_{wall}(\Delta) \left(\frac{L_\Delta(\Delta)}{\rho}\right)_{air}}, \quad (2.13)$$

where D_{wall}^{Fano} and D_{air}^{Fano} are the dose to the wall and air under the conditions described above, $\left(\frac{L_\Delta(E)}{\rho}\right)_{wall}$ and $\left(\frac{L_\Delta(E)}{\rho}\right)_{air}$ are the restricted mass-collision stopping powers in the wall and air, and $\Phi_{wall}(E)$ is the differential fluence of charged particles in the wall medium in the absence of a cavity. The use of Φ_{wall} in the calculation of both D_{wall}^{Fano} and D_{air}^{Fano} reflects the inherent assumption that the charged particle fluence spectrum in the cavity is the same as in the wall for $E > \Delta$. This assumption has been tested by including an additional correction factor in equation 2.12 to account for the perturbation of $\Phi_{wall}(E)$ by the cavity.^{25,57,68,73} Denoted here as K_{fl} , it may be expressed as

$$K_{fl} = \frac{K_{air}(1 - \bar{g}_{air}) \left(\frac{\bar{L}_\Delta}{\rho}\right)_{wall}^{air} \left(\frac{\bar{\mu}_{en}}{\rho}\right)_{air}^{wall}}{D_{air} K_{wall} K_{an} K_{comp} K} = \frac{(K_c)_{wall} \left(\frac{\bar{L}_\Delta}{\rho}\right)_{wall}^{air}}{D_{air}^{Fano}} \quad (2.14)$$

Whether a result of photon interactions in the cavity, or a difference between the composition of the wall and air (and, hence, scattering properties), calculations of

K_{fl} have shown that it is non-negligible at low photon energies⁵⁷ and for chambers with high-Z walls relative to air in ^{60}Co beams.^{25,68,73,74} Recalling the argument regarding having two parameters that are cavity-size dependent in section 2.1, the new stopping power ratio can be explicitly reformulated as

$$\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air} = \frac{D_{air}K_{wall}K_{an}K_{comp}K}{(K_c)_{air}} \left(\frac{\bar{\mu}_{en}}{\rho}\right)_{wall}^{air} = \frac{D_{air}^{Fano}}{(K_c)_{wall}}. \quad (2.15)$$

The same relationship is arrived at here as in equation 2.10, though with a full set of real ion chamber correction factors. As we will show, $\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air}$ can be expressed in terms of $\Phi_{wall}(E)$ and an energy deposition spectra, $\chi(E, \Omega)$, which is defined as the fraction of energy deposited in the cavity by a charged particle with energy E and direction $\vec{\Omega}$. The sections that follow present the derivation of $\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air}$ starting from the Boltzmann transport equation corresponding to conditions that apply to equations 2.10 and 2.15, namely the dose-to-air in the cavity due to an unattenuated, unscattered, broad-parallel photon beam (D_{air}^{Fano}). Comparisons are made with the Spencer-Attix formalism in the small cavity limit and both the potential applications and limitations of the new formalism are discussed in light of the assumptions made in the derivation.

2.2 The stopping power ratio as an effective source

The derivation of $\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air}$ is based on the concept of separating the true charged particle fluence $\Phi(E, \vec{\Omega}; \vec{x})$ in terms of the fluence in an infinite wall medium $[\Phi_{wall}(E, \vec{\Omega})]$

2.2. THE STOPPING POWER RATIO AS AN EFFECTIVE SOURCE

and a perturbation fluence $[\Phi_p(E, \vec{\Omega}; \vec{x})]$ due to the presence of the cavity:

$$\Phi(E, \vec{\Omega}; \vec{x}) = \Phi_{wall}(E, \vec{\Omega}) + \Phi_p(E, \vec{\Omega}; \vec{x}). \quad (2.16)$$

The variables $\vec{\Omega}$ and $\vec{x}$ represent angular distribution and position, respectively. $\Phi_{wall}(E, \vec{\Omega})$ is position-independent since it applies to the situation involving a homogeneous wall medium. By expressing $\Phi(E, \vec{\Omega}; \vec{x})$ as in equation 2.16, we may write D_{air}^{Fano} from equation 2.15 as

$$D_{air}^{Fano} = D_{wall}^{Fano} + D_p^{Fano}, \quad (2.17)$$

where

$$D_{wall}^{Fano} = \int_0^{E_0} dE \Phi_{wall}(E) F_\epsilon(E) \quad \text{and} \quad D_p^{Fano} = \int_0^{E_0} dE \Phi_p(E) F_\epsilon(E) \quad (2.18)$$

In equation 2.18, $F_\epsilon(E)$ is the energy per unit mass deposited in the cavity by charged particles with energy E via interactions with energy transfer less than ϵ . If the range of cut-off electrons with $E = \epsilon$ is small compared with the dimensions of the cavity, then

$$F_\epsilon(E) \approx \left(\frac{L_\epsilon(E)}{\rho} \right)_{air} \quad (2.19)$$

and

$$\begin{aligned} D_{wall}^{Fano} &= \int_0^{E_0} dE \Phi_{wall}(E) \left(\frac{L_\epsilon(E)}{\rho} \right)_{air} \\ &= \int_\epsilon^{E_0} dE \Phi_{wall}(E) \left(\frac{L_\epsilon(E)}{\rho} \right)_{air} + \epsilon \Phi_{wall}(\epsilon) \left(\frac{L_\epsilon(\epsilon)}{\rho} \right)_{air}, \end{aligned} \quad (2.20)$$

where $\epsilon\Phi_{wall}(\epsilon)\left(\frac{L_\epsilon(\epsilon)}{\rho}\right)_{air}$ accounts for the dose deposited by charged particles with $E < \epsilon$. Splitting the integral over $\Phi_{wall}(E)\left(\frac{L_\epsilon(E)}{\rho}\right)_{air}$ into the form shown above can be formally justified.¹⁹ For the calculation of D_p^{Fano} we replace $F_\epsilon(E)$ by an energy deposition spectra $\chi(E)$ for an effective source of charged particles, $S_{es}(E, \vec{\Omega}, \vec{x})$. Then D_p^{Fano} can be calculated according to

$$D_p^{Fano} = \int_0^{E_0} dE S_{es}(E, \vec{\Omega}, \vec{x}) \chi(E, \Omega). \quad (2.21)$$

One can think of $S_{es}(E)$ as a source that emits the fluence of charged particles $\Phi_p(E, \vec{\Omega}; \vec{x})$ that consists of positive and negative weights that, when added to $\Phi_{wall}(E, \vec{\Omega})$, yields the fluence of charged particles in the cavity, $\Phi(E, \vec{\Omega}; \vec{x})$. The task of derivating $S_{es}(E)$ from its corresponding transport equation is presented in the following section.

2.3 Derivation of the effective source

So far we have expressed D_{air}^{Fano} in terms of contributions from the charged particle fluence associated with a homogeneous wall medium and a fluence due to an effective source $S_{es}(E, \vec{\Omega}, \vec{x})$ that accounts for the presence of the cavity. This is the same approach used by Luo⁴⁷ in 1980 to calculate D_{air}^{Fano} with good success^{47,75} using an expression he derived that is unique from the one presented here. In 2011 a short and unheralded publication by Ren *et al.* also reported positive results using Luo's method.⁷⁶ We can obtain an expression for $S_{es}(E, \vec{\Omega}, \vec{x})$ in equation 2.21 in terms of $\Phi_{wall}(E, \vec{\Omega})$ from the respective transport equations for $\Phi(E, \vec{\Omega}; \vec{x})$, $\Phi_{wall}(E, \vec{\Omega})$, and $\Phi_p(E, \vec{\Omega}; \vec{x})$.

2.3.1 The transport equations

The transport equation for $\Phi(E, \vec{\Omega}; \vec{x})$, which includes “knock-on” electrons (δ -rays) but does not include charged particles set in motion by scattered photons, bremsstrahlung, annihilation photons or fluorescent x rays, is given as¹⁸

$$\begin{aligned} \vec{\Omega} \cdot \vec{\nabla} \Phi(E, \vec{\Omega}; \vec{x}) &= S(E, \vec{\Omega}, \vec{x}) \\ &+ \int_E^{E_0} dE' \int_{4\pi} d\Omega' \sigma(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}'; \vec{x}) \Phi(E', \vec{\Omega}'; \vec{x}) \\ &- \Phi(E, \vec{\Omega}; \vec{x}) \int_0^E dT \int_{4\pi} d\Omega' \sigma(E, T, \Omega'; \vec{x}), \end{aligned} \quad (2.22)$$

where $S(E, \vec{\Omega}, \vec{x})$ represents the source of charged particles that varies with position, $\vec{x}$, the first integral term sums ‘in-scattering’ along $\vec{\Omega}$ and the second term subtracts ‘out-scattering’ along $\vec{\Omega}'$, and $T = E' - E$. In this case,

$$\begin{aligned} S(E, \vec{\Omega}, \vec{x}) &= S_{wall}(E, \vec{\Omega}) \text{ if } \vec{x} \ni \text{wall}, \\ &= S_{air}(E, \vec{\Omega}) \text{ if } \vec{x} \ni \text{cavity}. \end{aligned} \quad (2.23)$$

$S_{wall}(E, \vec{\Omega})$ and $S_{air}(E, \vec{\Omega})$ are given by the product of the incident photon fluence and the differential cross-section for the production of charged particles with energy E and direction $\vec{\Omega}$ in the wall and in the cavity, respectively. Similarly, $\sigma(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}'; \vec{x})$ is the interaction probability per unit mass for a charged particle scattering from $(E', \vec{\Omega}')$ to $(E, \vec{\Omega})$, given as

$$\begin{aligned} \sigma(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}'; \vec{x}) &= \sigma_{wall}(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}') \text{ if } \vec{x} \ni \text{wall}, \\ &= \sigma_{air}(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}') \text{ if } \vec{x} \ni \text{cavity}. \end{aligned} \quad (2.24)$$

In the absence of a cavity, the charged particle fluence in the wall medium,

$\Phi_{wall}(E, \vec{\Omega})$, and its source, $S_{wall}(E, \vec{\Omega})$, are independent of $\vec{x}$ under Fano conditions.

We therefore have

$$\begin{aligned}
 \vec{\Omega} \cdot \vec{\nabla} \Phi_{wall}(E, \vec{\Omega}) &= S_{wall}(E, \vec{\Omega}) \\
 &+ \int_E^{E_0} dE' \int_{4\pi} d\Omega' \sigma_{wall}(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}') \Phi_{wall}(E', \vec{\Omega}') \\
 &- \Phi_{wall}(E, \vec{\Omega}) \int_0^E dT \int_{4\pi} d\Omega' \sigma_{wall}(E, T, \Omega') \\
 &= 0
 \end{aligned} \tag{2.25}$$

Likewise, the transport equation for $\Phi_p(E, \vec{\Omega}; \vec{x})$ is

$$\begin{aligned}
 \vec{\Omega} \cdot \vec{\nabla} \Phi_p(E, \vec{\Omega}; \vec{x}) &= S_{es}(E, \vec{\Omega}, \vec{x}) \\
 &+ \int_E^{E_0} dE' \int_{4\pi} d\Omega' \sigma(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}'; \vec{x}) \Phi_p(E', \vec{\Omega}'; \vec{x}) \\
 &- \Phi_p(E, \vec{\Omega}; \vec{x}) \int_0^E dT \int_{4\pi} d\Omega' \sigma(E, T, \Omega'; \vec{x})
 \end{aligned} \tag{2.26}$$

where $S_{es}(E, \vec{\Omega}, \vec{x}) = 0$ if $\vec{x}$ is outside the cavity.

2.3.2 The effective source

The effective source $S_{es}(E, \vec{\Omega}, \vec{x})$ introduced in equation 2.21 arises due to the difference between the photon and electron (and positron) scattering probabilities in the wall material and in air. Our goal is to obtain an expression for $S_{es}(E, \vec{\Omega}, \vec{x})$ in terms of $S(E, \vec{\Omega}, \vec{x})$ and the homogeneous fluence $\Phi_{wall}(E, \vec{\Omega})$. We begin by substituting equation 2.16 into equation 2.26 and combining with equation 2.22 to get:

$$S_{es}(E, \vec{\Omega}, \vec{x}) = S(E, \vec{\Omega}, \vec{x}) + I[\sigma, \Phi_{wall}], \tag{2.27}$$

where

$$\begin{aligned}
 I[\sigma, \Phi_{wall}] = & \int_E^{E_0} dE' \int_{4\pi} d\Omega' \sigma(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}'; \vec{x}) \Phi_{wall}(E', \vec{\Omega}') \\
 & - \Phi_{wall}(E, \vec{\Omega}) \int_0^E dT \int_{4\pi} d\Omega' \sigma(E, T, \Omega'; \vec{x}).
 \end{aligned} \tag{2.28}$$

Splitting each integral at $E = \epsilon$, we may write an expression for $I[\sigma_{air}, \Phi_{wall}]$ for $\vec{x}$ inside the cavity:

$$\begin{aligned}
 I[\sigma_{air}, \Phi_{wall}] = & \int_E^{E+\epsilon} dE' \sigma_{air}(E', E' - E) \Phi_{wall}(E') + \int_{E+\epsilon}^{E_0} dE' \sigma_{air}(E', E' - E) \Phi_{wall}(E') \\
 & - \Phi_{wall}(E) \int_0^\epsilon dT \sigma_{air}(E, T) - \Phi_{wall}(E) \int_\epsilon^E dT \sigma_{air}(E, T) \\
 & \boxed{\text{if } \vec{x} \ni \text{cavity}}.
 \end{aligned} \tag{2.29}$$

In order to simplify the notation, the dependence on $\vec{\Omega}$ has been ignored and all quantities affected are taken to be the integral over $d\Omega$.^a If we also ignore elastic scattering, which can be shown to be a valid approximation at ^{60}Co energies, then the charged particle scattering probability can be written in terms of the inelastic cross section per unit mass for the production of δ particles and atomic shell excitations, Σ^δ , and the cross section per unit mass for bremsstrahlung production, Σ^γ :

$$\sigma(E', E' - E) = \Sigma^\delta(E', E' - E) + \Sigma^\gamma(E', E' - E). \tag{2.30}$$

Equation 2.30 can be inserted into the second and fourth terms of equation 2.29, and the remaining terms of equation 2.29 can be combined by performing a change

^ae.g. $\sigma(E', E' - E) = \int_{4\pi} d\Omega' \sigma(E', E' - E, \vec{\Omega} \cdot \vec{\Omega}')$

2.3. DERIVATION OF THE EFFECTIVE SOURCE

of variables from E' to $T = E' - E$ in the first term,

$$\begin{aligned} I[\sigma_{air}, \Phi_{wall}] &= \int_{E+\epsilon}^{E_0} dE' \sigma_{air}(E', E' - E) \Phi_{wall}(E') - \Phi_{wall}(E) \int_{\epsilon}^E dT \sigma_{air}(E, T) \\ &\quad + \int_0^{\epsilon} dT [\Phi_{wall}(E + T) \sigma_{air}(E + T, T) - \Phi_{wall}(E) \sigma_{air}(E, T)]. \end{aligned} \quad (2.31)$$

The Fokker-Planck approximation⁷⁷ can then be applied with respect to T to this combined term assuming that ϵ is small enough in order for this approximation to be valid. The restrictions on ϵ will be discussed in section 2.6. Specifically, we assume $\Phi_{wall}(E + T) \sigma_{air}(E + T, T) \approx \Phi_{wall}(E) \sigma_{air}(E, T) + T \frac{\partial}{\partial E} [\Phi_{wall}(E) \sigma_{air}(E, T)]$, and therefore

$$\begin{aligned} I[\sigma_{air}, \Phi_{wall}] &= \int_{E+\epsilon}^{E_0} dE' \sigma_{air}(E', E' - E) \Phi_{wall}(E') - \Phi_{wall}(E) \int_{\epsilon}^E dT \sigma_{air}(E, T) \\ &\quad + \frac{\partial}{\partial E} \left[\Phi_{wall}(E) \int_0^{\epsilon} dT \sigma_{air}(E, T) T \right], \end{aligned} \quad (2.32)$$

where the integral in the square brackets defines the collisional stopping-power in air for a cut-off ϵ . Inserting equations 2.30 and 2.37 gives

$$\begin{aligned} S_{es}(E) &= S_{air}(E) + \frac{\partial}{\partial E} \left[\Phi_{wall}(E) \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{air} \right] \\ &\quad + \int_{E+\epsilon}^{E_0} dE' \Phi_{wall}(E') \Sigma_{air}^{\delta}(E', E' - E) - \Phi_{wall}(E) \Sigma_{air}^{\delta, tot}(E, \epsilon) \\ &\quad + \int_{E+\epsilon}^{E_0} dE' \Phi_{wall}(E') \Sigma_{air}^{\gamma}(E', E' - E) - \Phi_{wall}(E) \Sigma_{air}^{\gamma, tot}(E, \epsilon) \end{aligned} \quad (2.33)$$

where the relation $\Phi_{wall}(E) \int_{\epsilon}^E dT \sigma_{air}(E, T) = \Phi_{wall}(E) [\Sigma_{air}^{\delta, tot}(E, \epsilon) + \Sigma_{air}^{\gamma, tot}(E, \epsilon)]$ was used. Repeating the above process for the homogeneous transport equation (equa-

2.3. DERIVATION OF THE EFFECTIVE SOURCE

tion 2.25), we obtain

$$\begin{aligned}
0 = & S_{wall}(E) + \frac{\partial}{\partial E} \left[\Phi_{wall}(E) \left(\frac{L_\epsilon(E)}{\rho} \right)_{wall} \right] \\
& + \int_{E+\epsilon}^{E_0} dE' \Phi_{wall}(E') \Sigma_{wall}^\delta(E', E' - E) - \Phi_{wall}(E) \Sigma_{wall}^{\delta,tot}(E, \epsilon) \\
& + \int_{E+\epsilon}^{E_0} dE' \Phi_{wall}(E') \Sigma_{wall}^\gamma(E', E' - E) - \Phi_{wall}(E) \Sigma_{wall}^{\gamma,tot}(E, \epsilon)
\end{aligned} \tag{2.34}$$

If we assume ϵ is large compared to the binding energies of atomic electrons, then Σ^δ can be approximated by the Møller cross section. Thus,

$$\Sigma_{air}^\delta(E', E' - E) = \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \Sigma_{wall}^\delta(E', E' - E). \tag{2.35}$$

Repeating this process for the homogeneous transport equation for $\Phi_{wall}(E)$ and assuming that $\Sigma^\delta(E', E' - E)$ is given by the Møller cross sections, we combine equations 2.33-2.35 and have

$$\begin{aligned}
S_{es}(E) = & S_{air}(E) - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} S_{wall}(E) \\
& + \frac{\partial}{\partial E} \left\{ \Phi_{wall}(E) \left[\left(\frac{L_\epsilon(E)}{\rho} \right)_{air} - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_\epsilon(E)}{\rho} \right)_{wall} \right] \right\} \\
& + \Phi_{wall}(E) \left[\left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \Sigma_{wall}^{\gamma,tot}(E, \epsilon) - \Sigma_{air}^{\gamma,tot}(E, \epsilon) \right] \\
& + \int_{E+\epsilon}^{E_0} dE' \Phi_{wall}(E') \left[\Sigma_{air}^\gamma(E', E' - E) - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \Sigma_{wall}^\gamma(E', E' - E) \right],
\end{aligned} \tag{2.36}$$

2.3. DERIVATION OF THE EFFECTIVE SOURCE

where we have defined $\left(\frac{L_\epsilon(E)}{\rho}\right)_{air}$ and $\left(\frac{L_\epsilon(E)}{\rho}\right)_{wall}$ in the usual way:

$$\left(\frac{L_\epsilon(E)}{\rho}\right)_{air} = \int_0^\epsilon dT \sigma_{air}(E, T) T \quad \text{and} \quad \left(\frac{L_\epsilon(E)}{\rho}\right)_{wall} = \int_0^\epsilon dT \sigma_{wall}(E, T) T. \quad (2.37)$$

We may split equation 2.35 and write $S_{es}(E)$ as

$$S_{es}(E) = \begin{cases} S_0(E) + S_\delta(E) + S_\gamma(E), & \text{if } E \geq \epsilon \\ S_{air}(E), & \text{if } E < \epsilon, \end{cases} \quad (2.38)$$

where

$$\begin{aligned} S_0(E) &= S_{air}(E) - \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} S_{wall}(E) \\ S_\delta(E) &= \frac{\partial}{\partial E} \left\{ \Phi_{wall}(E) \left[\left(\frac{L_\epsilon(E)}{\rho}\right)_{air} - \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} \left(\frac{L_\epsilon(E)}{\rho}\right)_{wall} \right] \right\} \\ S_\gamma(E) &= \Phi_{wall}(E) \left[\left(\frac{\bar{Z}}{A}\right)_{wall}^{air} \Sigma_{wall}^{\gamma, tot}(E, \epsilon) - \Sigma_{air}^{\gamma, tot}(E, \epsilon) \right] \\ &\quad + \int_{E+\epsilon}^{E_0} dE' \Phi_{wall}(E') \left[\Sigma_{air}^\gamma(E', E' - E) - \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} \Sigma_{wall}^\gamma(E', E' - E) \right]. \end{aligned}$$

In equation 2.38, differences between the wall and air are broken down into:

- $S_0(E)$, which accounts for differences in photon scattering properties between the wall and cavity materials,
- $S_\delta(E)$, which accounts for differences in inelastic scattering properties between the wall and cavity materials, and
- $S_\gamma(E)$, which accounts for differences in bremsstrahlung yield between the wall and cavity materials.

2.4 Expression for the stopping power ratio

To obtain D_{air}^{Fano} recall equations 2.17, 2.20, and 2.21. Having D_{wall}^{Fano} in hand, the expression for D_p^{Fano} can be obtained by inserting equation 2.36 into 2.21, giving

$$\begin{aligned}
 D_p^{Fano} = & \int_0^{E_0} dES_{air}(E)\chi(E) - \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} \int_{\epsilon}^{E_0} dES_{wall}(E)\chi(E) \\
 & + \int_{\epsilon}^{E_0} dE \frac{\partial}{\partial E} \left\{ \Phi_{wall}(E) \left[\left(\frac{L_{\epsilon}(E)}{\rho}\right)_{air} - \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} \left(\frac{L_{\epsilon}(E)}{\rho}\right)_{wall} \right] \right\} \chi(E) \\
 & + \int_{\epsilon}^{E_0} dES_{\gamma}(E)\chi(E).
 \end{aligned} \tag{2.39}$$

We only integrate from ϵ to E_0 over $S_0(E)$, $S_{\delta}(E)$ and $S_{wall}(E)$ in the above expression since $S_{es}(E) = S_{air}(E)$ for $E < \epsilon$.

First we split the integration limits of the second term of equation 2.39 as

$$\left(\frac{\bar{Z}}{A}\right)_{wall}^{air} \int_{\epsilon}^{E_0} dES_{wall}(E)\chi(E) = \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} [\int_0^{E_0} dES_{wall}(E)\chi(E) - \int_0^{\epsilon} dES_{wall}(E)\chi(E)].$$

Then, adding the result of this to the expression for D_{wall}^{Fano} in equation 2.20 gives

$$\begin{aligned}
 D_{air}^{Fano} = & \int_{\epsilon}^{E_0} dE \Phi_{wall}(E) \left(\frac{L_{\epsilon}(E)}{\rho}\right)_{air} + \epsilon \Phi_{wall}(\epsilon) \left(\frac{L_{\epsilon}(\epsilon)}{\rho}\right)_{air} \\
 & + \int_0^{E_0} dES_{air}(E)\chi(E) - \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} \left[\int_0^{E_0} dES_{wall}(E)\chi(E) - \int_0^{\epsilon} dES_{wall}(E)\chi(E) \right] \\
 & + \int_{\epsilon}^{E_0} dE \frac{\partial}{\partial E} \left\{ \Phi_{wall}(E) \left[\left(\frac{L_{\epsilon}(E)}{\rho}\right)_{air} - \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} \left(\frac{L_{\epsilon}(E)}{\rho}\right)_{wall} \right] \right\} \chi(E) \\
 & + \int_{\epsilon}^{E_0} dES_{\gamma}(E)\chi(E).
 \end{aligned} \tag{2.40}$$

We note that $\chi(E) \approx E$ for $E < \epsilon$ (i.e. a charged particle will deposit all of its energy in the cavity below this threshold), and so we may approximate $\int_0^{\epsilon} dES_{wall}(E)\chi(E)$ as

2.4. EXPRESSION FOR THE STOPPING POWER RATIO

$\int_0^\epsilon dE S_{wall}(E)E$. We also assume that $\epsilon \Phi_{wall}(\epsilon) \left(\frac{L_\epsilon(\epsilon)}{\rho} \right)_{air} = \epsilon \Phi_{wall}(\epsilon) \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_\epsilon(\epsilon)}{\rho} \right)_{wall}$ since the fraction of energy lost as bremsstrahlung is negligible at low energies. Therefore,

$$\begin{aligned} D_{air}^{Fano} = & \int_0^{E_0} dE \chi(E) \left[S_{air}(E) - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} S_{wall}(E) \right] + \int_\epsilon^{E_0} dE S_\gamma(E) \chi(E) \\ & + \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left[\epsilon \Phi_{wall}(\epsilon) \left(\frac{L_\epsilon(\epsilon)}{\rho} \right)_{wall} + \int_0^\epsilon dE S_{wall}(E)E \right] + \int_\epsilon^{E_0} dE \left\{ \Phi_{wall}(E) \left(\frac{L_\epsilon(E)}{\rho} \right)_{air} \right. \\ & \left. + \frac{\partial}{\partial E} \left[\Phi_{wall}(E) \left(\left(\frac{L_\epsilon(E)}{\rho} \right)_{air} - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_\epsilon(E)}{\rho} \right)_{wall} \right) \right] \chi(E) \right\}. \quad (2.41) \end{aligned}$$

It follows from integration by parts of the final term that

$$\begin{aligned} & \int_\epsilon^{E_0} dE \frac{\partial}{\partial E} \left[\Phi_{wall}(E) \left(\left(\frac{L_\epsilon(E)}{\rho} \right)_{air} - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_\epsilon(E)}{\rho} \right)_{wall} \right) \right] \chi(E) = \\ & \quad \Phi_{wall}(E) \left[\left(\frac{L_\epsilon(E)}{\rho} \right)_{air} - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_\epsilon(E)}{\rho} \right)_{wall} \right] \chi(E) \Big|_\epsilon^{E_0} \\ & \quad - \int_\epsilon^{E_0} dE \left\{ \Phi_{wall}(E) \left[\left(\frac{L_\epsilon(E)}{\rho} \right)_{air} - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_\epsilon(E)}{\rho} \right)_{wall} \right] \right\} \frac{\partial \chi(E)}{\partial E}. \quad (2.42) \end{aligned}$$

Since bremsstrahlung production is negligible for $E < \epsilon$, and since $\chi(E) \approx 0$ at $E = E_0$, $\Phi_{wall}(E) \left[\left(\frac{L_\epsilon(E)}{\rho} \right)_{air} - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_\epsilon(E)}{\rho} \right)_{wall} \right] \chi(E) \Big|_\epsilon^{E_0} \approx 0$. Exploiting the relation between Møller cross sections for different materials, and assuming negligible energy loss by high-energy charged particles, we insert equation 2.42 into 2.41 and

D_{air}^{Fano} becomes

$$\begin{aligned}
D_{air}^{Fano} = & \int_{\epsilon}^{E_0} dE \Phi_{wall}(E) \left\{ \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{air} [1 - \chi'(E)] + \chi'(E) \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{wall} \right\} \\
& + \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left[\epsilon \Phi_{wall}(\epsilon) \left(\frac{L_{\epsilon}(\epsilon)}{\rho} \right)_{wall} + \int_0^{\epsilon} dE S_{wall}(E) E \right] \\
& + \int_0^{E_0} dE \chi(E) \left[S_{air}(E) - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} S_{wall}(E) \right] \\
& + \int_{\epsilon}^{E_0} dE S_{\gamma}(E) \chi(E),
\end{aligned} \tag{2.43}$$

where $\chi'(E) = \frac{\partial \chi(E)}{\partial E}$. The final expression for $\left(\frac{\bar{L}_{\epsilon}}{\rho} \right)_{wall}^{air}$ can then be obtained by dividing by $(K_c)_{wall} = \Psi_0 \left(\frac{\bar{\mu}_{en}}{\rho} \right)_{wall}$. In the above equation, the first term is analogous to the Spencer-Attix result for the dose-to-air without the track-end term, and with $\chi'(E) = 0$. The second term represents the contribution to D_{air}^{Fano} from track-ends, while the third term results from the difference between the photon scattering probabilities of the wall and air. The last term accounts for differences in bremsstrahlung yield between the wall and cavity but is negligible for the material and cavity size combinations of interest at ^{60}Co energies and lower.

2.5 Results

2.5.1 Small cavities and the convergence to the Spencer-Attix stopping-power ratio

The expression for D_{air}^{Fano} given in equation 2.43 approaches the Spencer-Attix formalism when the following conditions are met:

- Photo-absorption and pair production can be neglected and binding effects in Compton scattering are negligible (i.e. the Klein-Nishina cross section may be used). Therefore, $S_{air}(E) \approx \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} S_{wall}(E)$ for all energies, and

$$\int_0^{E_0} dE \chi(E) \left[S_{air}(E) - \left(\frac{\bar{Z}}{A}\right)_{wall}^{air} S_{wall}(E) \right] \approx 0. \quad (2.44)$$

- Bremsstrahlung production can be neglected:

$$\int_{\epsilon}^{E_0} dE S_{\gamma}(E) \chi(E) \approx 0. \quad (2.45)$$

- The cavity is sufficiently small such that the energy deposition spectra, $\chi(E)$ is given by^{17, 18, 78}

$$\begin{aligned} \chi(E) &= \Delta \text{ if } E > \Delta, \\ &= E \text{ if } E \leq \Delta, \end{aligned} \quad (2.46)$$

where Δ takes the place of ϵ since it depends on cavity size, and since ϵ is used to specify $\Phi_{wall}(E)$ rather than a property of the cavity.

These conditions are approximately satisfied for ^{60}Co beams incident on ion chambers with small cavities and air equivalent wall materials. Cavities are ‘small’ if their dimensions are small relative to the range of charged particles. Using the above approximations, equation 2.43 reduces to

$$D_{air}^{Fano} = \int_{\Delta}^{E_0} dE \Phi_{wall}(E) \left(\frac{L_{\Delta}(E)}{\rho} \right)_{air} + \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left[\Delta \Phi_{wall}(\Delta) \left(\frac{L_{\Delta}(\Delta)}{\rho} \right)_{wall} + \int_0^{\Delta} dE S_{wall}(E) E \right]. \quad (2.47)$$

The second term in the above equation converges to the track-end term in the Spencer-Attix formalism since bremsstrahlung production is negligible for $E < \Delta$ and $\Delta\Phi_{wall}(\Delta)\left(\frac{L_\Delta(\Delta)}{\rho}\right)_{wall} \gg \int_0^\Delta dES_{wall}(E)E$. In other words,

$$\left(\frac{\bar{Z}}{\bar{A}}\right)_{wall}^{air} \left[\Delta\Phi_{wall}(\Delta)\left(\frac{L_\Delta(\Delta)}{\rho}\right)_{wall} + \int_0^\Delta dES_{wall}(E)E \right] \approx \Delta\Phi_{wall}(\Delta)\left(\frac{L_\Delta(\Delta)}{\rho}\right)_{wall}^{air}. \quad (2.48)$$

Inserting equation 2.48 into equation 2.47 and dividing by D_{wall}^{Fano} gives $\left(\frac{\bar{L}_\Delta}{\rho}\right)_{wall}^{air}$, and so $\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air}$ converges to $\left(\frac{\bar{L}_\Delta}{\rho}\right)_{wall}^{air}$ in the small cavity limit.

2.5.2 Large cavity sizes and convergence to $\left(\frac{\bar{\mu}_{en}}{\rho}\right)_{wall}^{air}$

A cavity is ‘large’ if the dimensions are large relative to the range of charged particles.

In this limit, $\chi(E) = E$ for all E and so $\chi'(E) = 1$. Thus, D_{air}^{Fano} reduces to

$$\begin{aligned} D_{air}^{Fano} &\approx \left(\frac{\bar{Z}}{\bar{A}}\right)_{wall}^{air} \left[\int_\epsilon^{E_0} dE\Phi_{wall}(E)\left(\frac{L_\epsilon(E)}{\rho}\right)_{wall} + \epsilon\Phi_{wall}(E)\left(\frac{L_\epsilon(E)}{\rho}\right)_{wall} \right. \\ &\quad \left. + \int_0^\epsilon dES_{wall}(E)E \right] + \int_0^{E_0} dES_\gamma(E)E \\ &= \Psi_0\left(\frac{\bar{\mu}_{en}}{\rho}\right)_{air}. \end{aligned} \quad (2.49)$$

Dividing by $(K_c)_{wall}$, which is $\Psi_0\left(\frac{\bar{\mu}_{en}}{\rho}\right)_{wall}$, we see that $\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air}$ converges to $\left(\frac{\bar{\mu}_{en}}{\rho}\right)_{wall}^{air}$ in the large cavity limit.

2.5.3 An analytical expression for the fluence correction factor, K_{fl}

It follows from equation 2.14 that D_{air}^{Fano} is directly proportional to $A_{fl}\left(\frac{\bar{L}_\Delta}{\rho}\right)_{wall}^{air}$, where $A_{fl} = \frac{1}{K_{fl}}$. Assuming that $\left(\frac{\bar{Z}}{\bar{A}}\right)_{wall}^{air} \epsilon\Phi_{wall}(\epsilon)\left(\frac{L_\epsilon(\epsilon)}{\rho}\right)_{wall} \approx \epsilon\Phi_{wall}(\epsilon)\left(\frac{L_\epsilon(\epsilon)}{\rho}\right)_{air}^{air}$,

one can arrive at an analytical expression for A_{fl} given as

$$\begin{aligned}
A_{fl} = 1 &+ \int_{\epsilon}^{E_0} dE \chi'(E) \Phi_{wall}(E) \left[\left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{wall} - \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{air} \right] \\
&+ \int_0^{E_0} dE \chi(E) \left[S_{air}(E) - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} S_{wall}(E) \right] \\
&+ \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \int_0^{\epsilon} dE S_{wall}(E) E + \int_{\epsilon}^{E_0} dE S_{\gamma}(E) \chi(E).
\end{aligned} \tag{2.50}$$

This fluence correction could be applied to existing Spencer-Attix cavity theory to correct for the fluence perturbation by the presence of the cavity when using non-radiologically equivalent chamber materials, as well as at low incident photon energies, as long as $\epsilon = \Delta$. Using the novel cavity theory formalism introduced above would arrive at the same result, however, with much less computational input than using Spencer-Attix plus equation 2.50. So there is no benefit using equation 2.50 and Spencer-Attix, except to use equation 2.50 to provide clues about how inaccurate using the Spencer-Attix $\left(\frac{\bar{L}_{\Delta}}{\rho} \right)_{wall}^{air}$ approach is expected to be.

2.6 Summary

The expression for dose to an air-filled cavity (D_{air}^{Fano}) given by equation 2.43 depends on several quantities that also make up the Spencer-Attix formalism. These include the source-dependent, unperturbed fluence of charged particles in the medium ($\Phi_{wall}(E)$ in the case of the air kerma formalism given by equation 2.12), and the mass-restricted stopping powers of the medium and cavity $\left[\left(\frac{L_{\epsilon}(E)}{\rho} \right)_{wall} \text{ and } \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{air} \right]$. As with Spencer-Attix cavity theory, there is nothing restricting the application of equation 2.43 to in-phantom dosimetry problems provided attenuation, scatter, and divergence of the source – $S(E, \vec{\Omega}, \vec{x})$ – are accounted for in the calculation of $\Phi_{wall}(E)$.

Despite the similarities between equation 2.43 and the Spencer-Attix formulation, and even though the former converges to the latter in the small cavity limit, it differs from the latter in several ways. First, and most importantly, equation 2.43 does not rely on the ambiguous choice of a cavity-size dependent quantity analogous to the energy threshold Δ in the Spencer-Attix stopping power ratio. Instead, a new parameter ϵ is chosen such that in the charged particle energy range, bremsstrahlung production remains negligible. Restrictions on the value of ϵ are discussed in more detail in section 2.6.1. Additionally, the cavity-size dependence in equation 2.43, as we will show in chapter 5, is contained in the energy deposition function, $\chi(E)$. This quantity can be calculated with a simple and fast Monte Carlo calculation only once as it depends on the cavity and surrounding medium, and is independent of the incident photon source. The same is not true of the Spencer-Attix parameter Δ , which has been shown to be dependent on cavity size, surrounding material composition, and the incident beam energy.^{20,22,25,26} By accounting for the size and shape of the cavity through the direct calculation of $\chi(E)$, energy deposition by charged particles is treated explicitly - i.e., no assumptions are made about energy deposition. As well, material and cavity-size dependence is decoupled from the lower-bound threshold energy, ϵ , and the incident beam energy. The cavity-size dependence captured in $\chi(E)$ should reduce or even eliminate the need for additional fluence correction factors, such as the K_{fl} in the air kerma formalism (equation 2.14), or P_{fl} in the original formulation of k_Q . The former is explored explicitly in chapter 5.

Another distinguishing feature of equation 2.43 is the removal of Bragg-Gray conditions. Since perturbations to the charged particle fluence $\Phi_{wall}(E)$ are explicitly treated through the fictitious perturbation fluence, $\Phi_p(E)$, there are no explicit restrictions on cavity size and thus no requirement that the cavity be a Bragg-Gray

cavity. The liberation of primary charged particles within the cavity is also permitted in the formalism presented here, even though it also violates the second Bragg-Gray condition. We note that the second Bragg-Gray condition is effectively lifted when the radiological properties of the cavity and surrounding medium are similar,^{26,79} as can be the case for air-filled cavities surround by low-Z wall materials in high-energy photon fields. The implication of removing the two Bragg-Gray conditions is that equation 2.43 is potentially applicable over a wider range of cavity sizes, cavity wall materials, and incident beam energies. The accuracy of this formalism over broad ranges of these three variables is explored in the context of the air kerma formalism in chapter 5.

2.6.1 Restrictions on ϵ

While equation 2.43 is potentially applicable over a broader range of physical conditions, its application is not without restrictions. In particular, the parameter ϵ is constrained, owing to assumptions made throughout the derivation of equation 2.43, as follows:

- ϵ must be small enough to justify the Fokker-Planck approximation applied in equation 2.36.
- ϵ must be small enough such that bremsstrahlung production for $E \leq \epsilon$ can be neglected.
- ϵ must be small enough such that the ranges of charged particles with $E \leq \epsilon$ are small relative to the dimensions of the cavity.
- ϵ must be large relative to the binding energies of atomic electrons such that

Σ^δ can be approximated by the Møller and Bhabha cross sections.^b

In endeavoring to compute numerical results for equation 2.43, it is important to recognize that ϵ represents the lowest kinetic energy of charged particles tracked (and created) in a Monte Carlo simulation. Accuracy is generally ensured when tracking charged particles to the lowest possible kinetic energy, typically 1 keV, as that will limit the scoring of residual energy deposition at the incorrect locations. Such a low value also meets the first three restrictions listed above, but might not be appropriately large enough to assume negligible effects due to binding energies.

2.6.2 General application of a generalized stopping power ratio

In chapter 5 we describe a method of applying equation 2.43 to the stopping power ratio as defined in the air kerma formalism. Similar processes can be followed to calculate and interpret cavity doses for detectors at depth in a phantom. In addition to calculations of $\Phi_{wall}(E)$, values of $\chi(E)$, $S_{wall}(E)$, and $S_{air}(E)$ are needed to yield a result $\left(\int_{\epsilon}^{E_0} dE S_{\gamma}(E) \chi(E)\right)$ is assumed to be negligible). This computational overhead contrasts with Bragg-Gray, Spencer-Attix, and Burlin cavity theories, which are comparably straightforward mathematically but are conceptually more ambiguous. The quantity $\chi(E)$ is characteristic of a particular chamber/detector design and can be computed over the entire energy range of its intended use. The quantities $\Phi_{wall}(E)$, $S_{wall}(E)$, and $S_{air}(E)$ are all properties of the incident source, cavity medium (*e.g.* air) and surrounding medium (*e.g.* wall). The calculation of $S_{wall}(E)$ and $S_{air}(E)$ is obtained from a routine Monte Carlo simulation that is in addition to the calculation

^bFrom equation 2.35, Σ^δ is the inelastic cross section per unit mass for the production of δ particles and atomic shell excitations.

of $\Phi_{wall}(E)$. We speculate that the effort involved in calculating these quantities is worth the potential increase in accuracy. This approach also avoids laborious methods for determining appropriate quantities that account for cavity size effects in other formalisms.

Chapter 3

The EGSnrc Monte Carlo code system

3.1 Introduction

The Electron-Gamma-Shower code system maintained by the National Research Council of Canada (**EGSnrc**) is a general-purpose code package for the Monte Carlo simulation (this method will be covered in section 3.1.1) of the coupled transport of electrons and photons in constructed geometries.⁸⁰⁻⁸² Simulations can be run for particles with kinetic energies as low as 1 keV up to several hundred GeV. This latest iteration includes many updates and improvements over the original **EGS** system⁸³ and is possibly the gold standard in medical radiation physics applications. The accuracy has been reported at 0.1% with respect to the internal cross-sections and geometry definitions used in calculating the response of an ion chamber.⁸¹

Types of particle interactions modelled for photons include the photoelectric effect, coherent (Rayleigh) scattering, incoherent (Compton) scattering, pair – or triplet –

production (if the incident energy is sufficient), and photonuclear interactions.^{84–86} **EGSnrc** also models the after-effects of some of the previously mentioned processes, like characteristic x-ray production, Auger electrons, positron annihilation, and electron-nucleus interactions like Bremsstrahlung radiation. The next section will introduce the Monte Carlo simulation process.

3.1.1 Monte Carlo simulations of radiation transport

The Monte Carlo method was created as “a statistical approach to the study of differential equations”.⁸⁷ To apply this method to a physical situation the problem must be formulated in mathematical terms, usually as a system of equations in a complex situation. In the specific case of simulating the transport of ionizing radiation through matter, and interaction with media, the interaction cross-sections, stopping powers, scattering powers and other material data are required in order to sample at random. The Monte Carlo method uses a random number generator and the appropriate probability distributions to estimate a parameter of interest. By simulating many independent histories, each estimating the parameter of interest, the expectation value and statistical uncertainty (the standard deviation of the distribution of estimates) are calculated.

As a simple example of the process, the steps a photon will take as it traverses a medium are described. The photon will be assigned an initial energy, by sampling the source spectrum distribution, and a direction in relation to the geometry of interest. A random number generator using the total photon cross-section data appropriate for the energy and medium is used to determine the path-length traversed through the geometry before an interaction. At the end of the path the probabilities of the various types of interactions in the medium are normalized so that their cumulative

sum is one. Each interaction is assigned an appropriate portion of the range between zero and one and a newly generated uniform random number chooses the interaction type. Further outcomes of the interaction (how energy is conserved, directions of particles) are also sampled from the respective probability distributions governing those processes. If the result of the interaction creates one or more additional particles, they are set aside on a ‘stack’ for later processing. If the original photon still exists after the interaction, possibly with a lower energy and direction, a new path-length will be determined. This process repeats until the photon leaves the region of interest or its energy falls below a predetermined threshold. Each primary particle that is simulated, in this case a photon, is a ‘history’. This type of modelling is called event-by-event transport.⁸⁸

Another type of radiation transport simulation applied to transport of charged particles is the condensed-history (CH) technique.⁸⁹ Since it is normal to simulate a large number of histories to reduce the statistical uncertainty on the parameter of interest, the calculation time can be very long. This is especially true when scoring physical quantities that accumulate slowly (*e.g.* small fractional energy losses). Additionally, in the simulation of energetic charged particles, like electrons, many hundreds of thousands of interactions may occur that create secondary particles that also create tertiary particles, and so on. Due to the large amount of collisions being simulated the previously described event-by-event modelling becomes prohibitively long because of limited computing power. In the CH method, many transport and collision steps are modelled in a single charged particle step using multiple scattering theories.^{90,91} It has been shown that this simplification is able to match the accuracy of event-by-event radiation transport while greatly increasing the efficiency.⁹² The Monte Carlo software used in this investigation uses the CH technique.

3.2 EGSnrc overview

User codes are available for **EGSnrc** which facilitate the calculation of quantities of interest from the simulation of particle transport in geometries depicting experimental measurements. There are codes specifically for modelling linear accelerators (**BEAMnrc**),⁹³ codes for dose calculation in spherical and cylindrical geometries (**CAVRZnrc**, **SPRRZnrc**, **DOSErZnrc**),³⁰ rectilinear (**DOSEXYZnrc**),⁹⁴ and user defined geometries (**cavity**),⁹⁵ a code for particle fluences in cylindrical geometries (**FLURZnrc**)³⁰ and stopping power ratios (**SPRRZnrc**),³⁰ and a code to calculate the radiative yield (**g**).⁸²

3.2.1 Dosimetric quantities of interest

In chapter 4 the dose to the cavity of a parallel plate ion chamber, and the dose to a uniform medium, are calculated using both the cylindrical geometry (**CAVRZnrc**) and user defined geometry (**cavity**) codes. **CAVRZnrc** is a FORTRAN-based user code that enables the calculation of dose restricted to cylindrical symmetric volumes of various materials with common radii. The **cavity** code is C++ based and has a very flexible geometry package that allows users to define complex geometries. These two user codes have very different input file structures but calculate the same quantities.

In chapter 5 the components of the formalism introduced in chapter 2 are calculated using the codes presented in table 3.1. The fluences of charged particles passing through the cavity of a parallel plate ion chamber, as well as in a uniform medium, are calculated with **FLURZnrc**. Track end terms and the energy distribution of low energy charged particles are calculated in both **FLURZnrc** and **SPRRZnrc** user codes. The amount of energy an electron, with an initial position and direction in a plane-parallel ion chamber, will deposit in that cavity ion chamber was calculated

with **cavity**. This user code specifically allowed for the source of electrons to be created inside the cavity of the chamber with random energies and directions. The user codes used to investigate these dosimetric quantities are listed in table 3.1.

Table 3.1: **EGSnrc** codes used to investigate dosimetric quantities.

User-code	Purpose
CAVRZnrc	Calculates the dose to the cavity of an ion chamber per unit incident fluence. Restricted to cylindrical chamber styles.
cavity	Calculates the dose to an arbitrary geometry per incident fluence. It is much more flexible than its CAVRZnrc predecessors.
SPRRZnrc	Calculates the Spencer-Attix ratio of spectrum-averaged mass restricted stopping-powers for two materials.
FLURZnrc	Calculates the fluence of photons or charged particles (electrons and positrons) in a cylindrical geometry. Distinguishes between primary and secondary particles.
g	Calculates values of $\left(\frac{\bar{\mu}_{\text{en}}}{\rho}\right)$ for a photon source. Calculates $\bar{g}$, which is the fraction of kinetic energy transferred from photons to charged particles that is subsequently lost to radiative processes.

3.2.2 Physical processes simulated

An important feature of the novel cavity theory derivation presented in section 2.1.1 is that the effects of attenuation and scatter have been removed. Therefore, the input parameters of the various user codes have been chosen or modified so that the simulations could run under these artificial conditions. This mode is referred to as photon regeneration, designed to simulate the Fano conditions that were introduced in section 2.1. When calculating dosimetric quantities with photon regeneration enabled, the energy, position, and direction of incident photons are noted before an interaction takes place. Any scattered photons after the interaction are discarded and a new photon with the pre-interaction properties is regenerated at that location. Other processes discarded include relaxation processes, bremsstrahlung radiation, and positron annihilation photons. This removes the effects of attenuation and scatter and ensures true charged particle equilibrium beyond the depth of full charged particle build up. Both **CAVRZnrc** and **cavity** have two calculation modes which achieve this situation. The first is the previously mentioned photon regeneration and the second is a full chamber dose simulation corrected by the A_{wall} parameter (see section 2.1), which is calculated concurrently.

3.2.3 Simulation parameters

The parameters input into an **EGSnrc** simulation are grouped according to Monte Carlo, geometry, source, transport, media, and variance reduction headings. Monte Carlo inputs control the number of independent histories and the statistical accuracy of the simulation. Geometry inputs describe the regions of interest under which transport is to be simulated, and the particle type, energy, and orientation relative to the geometric inputs are defined by the source category. The transport parameters define

the types of interactions and the cross-section data from which to sample from. Media definitions include material specific data, which stopping powers should be used, and what threshold energies should be used for creating and transporting particles. Variance reduction techniques offer the ability to increase calculation efficiency, therefore decreasing the length of CPU time required, to achieve a given statistical uncertainty.

Transport parameters for both charged and uncharged particles in the majority of simulations in this research are shown in table 4.2 of the next chapter. These options allow calculations to be run with or without accounting for electron elastic scattering spin effects, Compton scattering and radiative corrections, triplet production, photoelectron angular sampling, and atomic relaxations. The energy cutoffs for creating particles, AE for electrons and AP for photons, and the energy cutoffs for transporting particles, ECUT for electrons and PCUT for photons, are varied in this research to test the accuracy of the new cavity theory formalism as well as compare it to Spencer-Attix cavity theory. The AE parameter is analogous to Δ and ϵ in equations 1.9 and 2.43, respectively, when $ECUT = AE$.

All the simulations used the XCOM photon cross-sections^{96–98} and restricted stopping powers from the National Institute of Standards and Technology (NIST) in the United States. These stopping powers include the density effect corrections published in the International Commission on Radiation Units Report (ICRU) 37.⁹⁹ There have been investigations into the correct mean excitation energy (I -value) to use for graphite; whether the ICRU value of 78 eV or the value from more recent publications of 87 eV.^{73,100} The I value recommended by the ICRU has been used in all of these calculations.

Chapter 4

Generation and validation of a library of calculated ion chamber doses for investigating cavity theories

4.1 Introduction

Cavity theories are foundational to the development and understanding of radiation dosimetry. Several cavity theories are in widespread use, but are based predominantly on theoretical frameworks and assumptions established in the mid-1950s and 1960s, as introduced in section [1.2](#). Owing to the computational tools available at the time, these early cavity theories reflect approximations and require modifications with calculated, or measured, correction factors to suit non-standard measurement conditions and detector types. As will be shown, detector response to ionizing ra-

diation are sensitive to a number of physical properties that are difficult to capture analytically in a cavity theory formalism (e.g. detector geometry, detector material composition, environmental conditions, correction factors to measured signals, etc.).

By necessity, correction factors are applied to cavity theory formalisms to account for non-ideal conditions (*e.g.* attenuation, scatter, source geometry, and detector material inhomogeneities). The correction factors are typically calculated using Monte Carlo methods as these calculations leave no uncertainty as to the material and geometry definitions. Further, when appropriately defined as a dose ratio, these corrections have been shown to be insensitive to the exact choice of transport parameters, certainly as applied to graphite chambers in ^{60}Co beams.³⁰

But there is growing interest in improved dosimetry at other, particularly low, energies in support of novel x-ray devices geared toward small animal irradiation, for example. At low energies the application of the popular cavity theories is made challenging due to the sensitivity to detector geometry and material, to the point of them being considered inapplicable to those situations.

The novel cavity theory presented in chapter 2 has yet to be investigated fully. Given the challenges associated with investigating the accuracy of cavity theories using experimental methods, particularly those related to the uncertainties in detector geometry and material composition, the next chapters explore the accuracy of the cavity theory introduced in chapter 2 using purely computational methods based on firmly established Monte Carlo codes. A necessary part of such an investigation is the generation of a reliable set of data by which we can benchmark novel cavity theories independent of experimental uncertainties. A data set covering a broad range of physical condition is presented here for bench-marking cavity theories using the Monte Carlo **EGSnrc** code base.⁸⁰

4.2 Materials and methods

4.2.1 Monte Carlo simulations

Simulation setup

Monte Carlo calculations of dose to an air cavity of an ion chamber free-in-air and dose to the uniform wall medium were performed using both **EGSnrc cavity** and **CAVRZnrc** user code bases. Both user codes were used to independently corroborate calculated doses. An idealized, cylindrically symmetric, pancake type ion chamber with no internal structure was created in both user codes with various wall materials and cavity heights. Cavity height refers to the distance between the front and back faces of the cavity walls perpendicular to the incident source (beam) of ionizing radiation. A stylized depiction of the cylindrically symmetric chamber is shown in Figure 4.1.

Broad-parallel photon beams were set perpendicular to the flat face of the chamber. Mono-energetic beams, ranging in energy from 0.05–1.25 MeV, and spectra for 120 kVp and ^{60}Co beams, were employed with beam radii equal to the outer radius of the chamber. Chamber walls were simulated using four materials: low Z beryllium and graphite (1.7 g/cm^3) and higher Z aluminum and copper. Internal **EGSnrc** material definitions were used in all simulations. Wall thicknesses were set to ensure full charged particle build up in the wall by calculating the continuous slowing down approximation (CSDA) range in each material and energy combination, as listed in Table 4.1. Full build-up refers to the range of the maximum energy electron that can be set in motion by a photon in the wall material, as calculated by the continuous slowing down approximation.

Table 4.1: Chamber wall thicknesses used to provide full buildup of charged particles for various incident photon beams. The wall thicknesses were created slightly larger than the maximum continuous slowing down approximation range.

Element	Chamber wall thickness in centimeters (cm) for incident photon beams of energy				
	0.05 (MeV)	120 kVp	0.30 (MeV)	1.25 (MeV)	^{60}Co
Beryllium	0.003	—	0.06	0.4	—
Graphite	0.003	0.014	0.06	0.4	0.41
Aluminum	0.003	—	0.05	0.3	—
Copper	0.0008	0.0036	0.02	0.1	0.1

Figure 4.1: Idealized pancake chamber schematic with no internal structure used for scoring dose. A homogeneous wall material surrounding a cavity filled with air.

The inner cavity radius was constant at 10 mm and the absorbed doses were calculated as a function of increasing cavity height (0.1 – 10 mm). The dose to homogeneous wall medium was calculated by replacing the air in the cavity with wall material. Two methods of dose scoring were employed: for the first method the dose deposited in the cavity was corrected by the fraction of photons which were scattered or attenuated by the wall, $D^{A_{wall}} = \frac{Dose}{A_{wall}}$. In the second method all dose-depositing photon interactions were regenerated with their original energy and direction before the scattered photons were discarded, D^{Fano} . Both $D^{A_{wall}}$ and D^{Fano} represent the dose to the cavity, whether filled with air or wall material, independent of the effects of attenuation and scatter of the incident primary beam by the chamber wall and cavity. Strictly speaking, D^{Fano} refers to the dose in a geometry of uniform composition (not necessarily uniform density), but it is used here to refer to the calculation method.

The rationale for using two scoring methods for the same quantity is the same as the rationale for using **cavity** and **CAVRZnrc** – an independent confirmation of the results.

Transport parameters

Dose simulations were run with the global AE and ECUT values (both displayed as the sum of particle rest mass energy plus kinetic energy), the lower cutoff for charged particle creation and the lower cutoff for charged particle transport, respectively, varying between 0.512, 0.514, and 0.521 MeV. The global AP and PCUT values, the lower cutoff for photon creation and the lower cutoff for photon transport, respectively, varied between 0.001, 0.003, and 0.01 MeV. AE and ECUT were set to the same value for all simulations, likewise for AP and PCUT. The upper total energy (rest plus kinetic) limits for charged particle transport (UE) and photon transport (UP) were set to 0.57 MeV for the 50 keV incident photon beam and to 0.82 MeV for the 300 keV and 120 kVp incident beams. The 1.25 MeV and ^{60}Co incident beam calculations kept the default UE and UP values of 2 MeV. To investigate the sensitivity of dose ratios on the choice of transport parameters, a complete set of ‘Simple’ simulations were completed. Deviations from the **EGSnrc** transport parameters laid out in⁸⁰ are shown in Table 4.2. The only variance reduction techniques employed in all simulations for **cavity** was *photon splitting* = 2 and for **CAVRZnrc** was *photon forcing* = on, with one interaction forced in the chamber wall. Calculated values of dose to air in the cavity ($D_{air}^{A_{wall}}$ or D_{air}^{Fano}) per incident fluence were normalized by the dose to a uniform wall material ($D_{wall}^{A_{wall}}$ or D_{wall}^{Fano}) calculated using a consistent set of interaction cross-sections, stopping powers, scattering powers, and transport parameters, as well as calculation method.

Table 4.2: **EGSnrc** Dose simulation transport parameters that were used to compare the ‘Full’ and ‘Simple’ dose ratio calculations.

Transport Parameter	Full	Simple
Brems cross sections	NRC	NRC
Photon cross sections	xcom	xcom
Compton cross sections	xcom	xcom
Bound Compton scattering	Simple	Simple
Triplet production	On	On
Rayleigh scattering	Off	Off
Radiative Compton corrections	On	Off
Spin effects	On	Off
Photoelectron angular sampling	On	Off
Atomic relaxations	On	Off

4.3 Results

4.3.1 Monte Carlo calculation of ion chamber response

The doses, D_{air} and D_{wall} , were simulated in combinations of four materials, seven cavity heights, three incident photon energies, three cutoff energies for the creation of particles (ECUT and PCUT), three cutoff energies for the transport of particles (AE and AP), two dose scoring methods, and two user codes. Individual statistical uncertainties on air cavity and uniform wall material doses were calculated to 0.04% or less in the majority of simulations, and the uncertainties of the dose ratios were 0.13% or less over all combinations simulated.

Figures 4.2 and 4.3 show representative samples of Monte Carlo calculated dose ratios, $\frac{D_{air}^{Fano}}{D_{wall}^{Fano}}$, comparing **cavity** and **CAVRZnrc** in a 1.25 MeV mono-energetic incident photon beam for chamber walls made of beryllium, graphite, aluminum, and copper. The dose ratios increase with increasing cavity size by 1.1% in beryllium and by 0.4% in graphite for the 1 keV transport cutoff. In aluminum and copper the dose ratios decrease with increasing cavity size by 3% and 8%, respectively for the 1 keV transport cutoff. Percent difference comparisons between the dose ratios calculated by **cavity** and **CAVRZnrc** are within 0.1% over the range of cavity heights simulated in beryllium and graphite. In aluminum and copper these dose ratios agree within 0.2% and 0.6%, respectively. The largest dose ratio disagreements were seen in the 1 keV transport cutoff in the smallest cavity sizes (0.1 and 0.2 mm), which are much smaller than any commercially available ion chamber.

Figure 4.2: Dose ratios of $\frac{D_{air}^{Fano}}{D_{wall}^{Fano}}$ for monoenergetic 1.25 MeV photons calculated by **cavity** and **CAVRZnrc** in beryllium and graphite wall materials. The transport cutoffs shown are for AE and ECUT (minus the particle rest mass energy), AP and PCUT.

Figure 4.3: Dose ratios of $\frac{D_{air}^{Fano}}{D_{wall}^{Fano}}$ for monoenergetic 1.25 MeV photons calculated by **cavity** and **CAVRZnrc** in aluminum and copper wall materials. The transport cutoffs shown are for AE and ECUT (minus the particle rest mass energy), AP and PCUT.

Dose ratio comparisons for a 0.3 MeV mono-energetic incident photon beam with the same simulation details as before were also consistent. The dose ratios increase with increasing cavity size by 1.7% in beryllium and by 0.7% in graphite for the 1 keV transport cutoff. In aluminum and copper the dose ratios decrease with increasing cavity size by 4% and 10%, respectively for the 1 keV transport cutoff. Percent difference comparisons between the dose ratios calculated by **cavity** and **CAVRZnrc** are within 0.1% over the range of cavity heights simulated in all materials.

For a 0.05 MeV mono-energetic incident photon beam the dose ratios increase with increasing cavity size by 22% in beryllium and by 11% in graphite for the 1 keV transport cutoff. In aluminum and copper the dose ratios decrease with increasing cavity size by 21% and 52%, respectively for the 1 keV transport cutoff. Percent difference comparisons between the dose ratios calculated by **cavity** and **CAVRZnrc** are within 0.3% over the range of cavity heights simulated in all materials. The simulations comparing $Fano$ to A_{wall} corrected dose ratios, and A_{wall} to A_{wall} , calculated in both codes showed agreement similar to the $Fano$ to $Fano$ comparison above for all three incident energies. The 120 kVp and ^{60}Co spectra were not used to compare **cavity** to **CAVRZnrc**, but will be used in chapter 5 to investigate the accuracy of the novel cavity theory formalism.

4.3.2 Simple versus full transport parameters

This section compares the dose ratio results simulated with the “Full” particle transport parameters outlined in Section 4.2, Table 4.2, to those obtained with the “Simple” transport. Either of the two simulation codes could have been used here, but **CAVRZnrc** $Fano$ calculations were chosen to simulate the simple dose ratios. The dose ratios were re-calculated using “Simple” transport parameters for all combina-

tions outlined in the previous section, 4.3.1. Figure 4.4 shows the $\frac{Simple}{Full}$ ratios (*i.e.* ratio of dose ratios) calculated using **CAVRZnrc** *Fano* conditions with an incident energy of 1.25 MeV and four materials. The copper chamber shows a difference between the simple dose ratio in the smallest cavity heights and lowest transport cutoffs, 1 and 3 keV. The three lighter-Z material ratios of dose ratios agree between transport parameters.

Figure 4.4: **CAVRZnrc** calculated ratios $\left(\frac{Simple}{Full}\right)$ of dose ratios $\left(\frac{D_{air}^{Fano}}{D_{wall}^{Fano}}\right)$ for a 1.25 MeV mono-energetic photon beam for three transport cutoff values.

For a 0.3 MeV mono-energetic photon beam the simple and full dose ratios for beryllium, graphite, and aluminum agree, but copper experiences about a 0.5–1% increase in simple dose ratio relative to the full dose ratio (Figure 4.5). The difference in dose ratios increases for the largest transport cutoff (kinetic energy 10 keV).

Figure 4.5: **CAVRZnrc** calculated ratios $\left(\frac{Simple}{Full}\right)$ of dose ratios $\left(\frac{D_{air}^{Fano}}{D_{wall}^{Fano}}\right)$ for a 0.3 MeV mono-energetic photon beam.

For a 0.05 MeV mono-energetic photon beam the beryllium simple dose ratio is underestimated by up to 10% lower, the graphite simple dose ratio is lower by up to

5%, the aluminum simple dose ratio is larger by up to 5%, and the copper simple dose ratio is larger by up to 34%. The largest transport cutoff (AE and ECUT) of 10 keV shows the worst agreement between simple and full transport (Figure 4.6).

Figure 4.6: **CAVRZnrc** calculated ratios $\left(\frac{Simple}{Full}\right)$ of dose ratios $\left(\frac{D_{air}^{Fano}}{D_{wall}^{Fano}}\right)$ for a 0.05 MeV mono-energetic photon beam and three charged particle transport cutoffs.

It is known that including atomic relaxations in the charged particle transport for low incident energy simulations is necessary to achieve calculated doses that accurately reflect experiments.¹⁰¹ However, we have not found published literature

showing the magnitude of this effect without atomic relaxations simulated. Figure 4.7 shows the ratio of dose ratios, with the only difference being the simulation of atomic relaxations, in all four materials for a 0.05 MeV mono-energetic photon beam and only the 1 keV transport cutoff. In beryllium and graphite there is a 3% and 2% reduction, respectively, in dose ratio across all cavity heights with atomic relaxations switched off, while aluminum and copper show a 3% and a 5–20% increase (increasing with cavity height), respectively, in dose ratio compared to simulating atomic relaxations.

Similar calculations comparing the effect of with-versus-without photoelectron angular sampling showed an unexpected result, as shown in Figure 4.8. Beryllium is most affected where the dose ratio decreases by more than 6% when not considering photoelectron angular sampling. Graphite shows a decrease in dose ratio of more than 3%. Aluminum and copper are less affected and show up to $\sim 2\%$ increases in the dose ratio. When increasing the incident photon energy to 0.3 MeV the only difference seen is when atomic relaxations are turned off in copper, shown in Figure 4.9. This effect dominates the difference between simple and full transport parameters seen in Figure 4.5 for copper walled chambers. Further investigations with radiative Compton corrections and spin effects did not result in observable dose ratio differences.

Figure 4.7: **CAVRZnrc** calculated ratios of dose ratios $\left(\frac{D^{Fano}_{air}}{D^{Fano}_{wall}}\right)$ highlighting the effect of simulating atomic relaxations for a 0.05 MeV mono-energetic photon beam and 1 keV transport cutoffs.

Figure 4.8: **CAVRZnrc** calculated ratios of dose ratios $\left(\frac{D_{air}^{Fano}}{D_{wall}^{Fano}}\right)$ highlighting the effect of simulating photoelectron angular sampling for a 0.05 MeV mono-energetic photon beam and 1 keV transport cutoffs.

Figure 4.9: **CAVRZnrc** calculated ratios of dose ratios ($\frac{D_{air}^{Fano}}{D_{wall}^{Fano}}$) highlighting the effect of simulating atomic relaxations for a 0.3 MeV mono-energetic photon beam and 1 keV transport cutoffs.

4.3.3 Rayleigh scattering in cavity

While building the library of dose ratios the *Rayleigh Scattering* transport parameter was turned on when simulating the **cavity** user-code *Fano*-calculated dose to wall medium, D_{wall}^{Fano} . This dose increased with increasing cavity size for the three energies investigated. The hallmark of a *Fano* dose is that the artificial charged particle equilibrium in a uniform medium leads to a constant dose independent of location and density variations throughout the medium.⁶⁹ The deviation from this expected behavior was most noticeable at lower incident photon energies. When the Rayleigh scattering transport parameter was turned off the dose behaved as a *Fano* dose should, as shown in Figure 4.10. This is most likely a bug specific to the **cavity** input-file choice *calculation type* = *Fano* as the A_{wall} corrected dose agreed with **CAVRZnrc** in both *Fano* and A_{wall} corrected doses. Since Rayleigh scattering does not contribute to energy deposition, and therefore neither to dose, there was no reason to simulate this interaction process under *Fano* conditions.

(a) 1.25 MeV

(b) 0.3 MeV

(c) 0.05 MeV

Figure 4.10: **Cavity** user-code calculated doses to copper wall medium for three mono-energetic incident photon beams [(a) 1.25 MeV, (b) 0.3 MeV, (c) 0.05 MeV]. The **cavity** user-code has a bug that calculates ion chamber response incorrectly when Rayleigh scattering is enabled along with ‘*calculation type = Fano*’ mode and is especially noticeable at lower incident energies.

4.4 Summary

The motivation behind these simulations was to create a library of dose ratios for the purpose of bench-marking novel cavity theories. Two Monte Carlo user-codes and two dose scoring methods were employed which independently confirmed that the calculated doses were consistent. Prior comparisons between **EGSnrc** calculations, using **CAVRZnrc** and **cavity** user-codes, and experimental measurements have established the accuracy of these calculations in the energy ranges examined here.¹⁰¹ Additionally, inconsistencies in the input parameters and the results were identified and accounted for. In general, these results helped define transport parameter boundaries and the requirements necessary for accurate dose calculations with **EGSnrc**. They also reveal the relative impact of various physical processes on relative ion chamber dose calculations as a function of incident beam energy, chamber material composition, and cavity size.

4.4.1 Monte Carlo user-code and dose scoring comparison

This set of data shows good agreement between the **cavity** and **CAVRZnrc** calculated ratio of doses for both D^{Fano} and $D^{A_{wall}}$ at all incident energies simulated. The choice of user-code or scoring option, D^{Fano} or $D^{A_{wall}}$, does not have an effect on the ratio of $\frac{D_{air}^*}{D_{wall}^*}$ (where * represents A_{wall} or $Fano$). Monte Carlo calculations of D_{air}^{Fano} in both **cavity** and **CAVRZnrc** take between ten minutes and seventeen hours for sub-0.05% dose uncertainties with the highest atomic number, smallest cavity size, and 1.25 MeV incident beam energy taking the longest. The same calculations of D_{wall}^{Fano} take three minutes to thirteen hours with the highest atomic number, smallest cavity size, and 0.05 MeV incident beam energy taking the longest. The **cavity** code, when combined with $Fano$ calculations and simulating Rayleigh scattering, has

a bug when calculating dose that is most apparent at low incident energies and in ‘larger’ (1–10 mm), wall-medium filled cavities. Caution should be exercised when using *calculation type* = **Fano**, or just use the A_{wall} corrected dose. Excluding Rayleigh scattering processes from the dose calculations under *Fano* conditions does not impact calculated results.

4.4.2 The effect of transport parameter choice on ion chamber cavity dose

Ion chamber cavity doses in graphite have been shown to be insensitive to variations in the details of particle transport using **EGSnrc** in ^{60}Co beams.³⁰ Our results for graphite in mono-energetic 1.25 MeV photon beams confirm those previous observations. The insensitivity to changes in transport parameters, dose scoring, and user-codes can be extended to beryllium, graphite, and aluminum in mono-energetic 1.25 MeV and 0.3 MeV photon beams, but does not hold for copper at 1.25 MeV and 0.3 MeV and all four materials at 0.05 MeV. At 0.05 MeV two transport parameters, atomic relaxations and photoelectron angular sampling, have large effects on calculated dose ratios– they are lower for low Z materials and larger in high Z materials. The atomic number (Z) of the wall is “low” if it is lower than the effective atomic number of the gas, in this case air, in the cavity, and “high” otherwise. In the **EGSnrc** manual, PIRS-701,⁸⁰ under *photoelectron angular sampling* Kawrakow notes:

The only application that I encountered until now where this option made a small difference was a big ion chamber (cavity size comparable with electron range) with high-Z walls in a low energy photon beam.

The range of effect for photoangular sampling can now be extended to small ion chambers with low-Z walls in low energy photon beams.

Chapter 5

Investigating the accuracy of the novel cavity theory formalism

5.1 Introduction

In the previous chapters a novel cavity theory formalism was introduced (chapter 2), the **EGSnrc** Monte Carlo simulation software was introduced (chapter 3), and this code base was used to establish a library of reference benchmark dose ratios using two codes (chapter 4). These provide the foundation to investigate the novel cavity theory formalism and probe its boundaries. In the past, a few historical cavity theory formalisms have been investigated very thoroughly and are ‘household names’ in dosimetry (*e.g.* Bragg-Gray, Spencer-Attix, Burlin)^{10,17,31} while others are relatively unknown (*e.g.* Ayala, Fu, Haider, Kearsley, Luo).^{47–50,75} The former are mathematically simple, easy to implement, and predict dose ratios very well under certain conditions as long as one has reasonable estimates regarding their non-physical parameters (Δ and $\mathbf{d}$). The latter are either too mathematically complex, or have been

shown to be less accurate than the former, or have not been thoroughly investigated. This chapter will determine whether the novel cavity theory can perform as well as Spencer-Attix at higher energies as well as investigate the lower bounds of accuracy. The hope is that this general cavity theory could be used to reformulate and unify dosimetry protocols over the full range of treatment beams, field sizes, and detector types of clinical relevance. This comes at the expense of an acceptable level of added complexity but with fewer simplifying assumptions and necessary correction factors (covered in sections 1.2.2 and 1.2.3).

Recall the formalism input parameters that will be Monte Carlo calculated from equation 2.43 on page 36:

$$\begin{aligned}
 D_{air}^{Fano} = & \int_{\epsilon}^{E_0} dE \Phi_{wall}(E) \left\{ \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{air} [1 - \chi'(E)] + \chi'(E) \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{wall} \right\} \\
 & + \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} \left[\epsilon \Phi_{wall}(\epsilon) \left(\frac{L_{\epsilon}(\epsilon)}{\rho} \right)_{wall} + \int_0^{\epsilon} dE S_{wall}(E) E \right] \\
 & + \int_0^{E_0} dE \chi(E) \left[S_{air}(E) - \left(\frac{\bar{Z}}{A} \right)_{wall}^{air} S_{wall}(E) \right] \\
 & + \int_{\epsilon}^{E_0} dE S_{\gamma}(E) \chi(E),
 \end{aligned} \tag{5.1}$$

where ϵ is the transport cutoff energy for creating and tracking charged particles, E_0 is the maximum incident photon energy, $\Phi_{wall}(E)$ is the charged particle slowing down dose spectra in the medium including secondary “knock-on” electrons liberated by charged particle collisional interactions, $\left(\frac{L_{\epsilon}(E)}{\rho} \right)_{air}$ and $\left(\frac{L_{\epsilon}(E)}{\rho} \right)_{wall}$ are the restricted mass collisional material stopping powers, $S_{air}(E)$ and $S_{wall}(E)$ are the initial charged particle spectra created by the incident source, $\chi(E)$ is the energy deposition spectra in the cavity, and $S_{\gamma}(E)$ is a source term accounting for the difference in bremsstrahlung yield between the cavity wall and gas, assumed here to be

dry air.

5.2 Methods

5.2.1 Monte Carlo calculations

The idealized pancake chamber presented in figure 4.1 on page 55 was implemented in the **EGSnrc** codes used to calculate parameters for the formalism given by equation 5.1. These include **FLURZnrc**, **cavity**, and **SPRRZnrc**.¹⁰² Calculations of D_{air}^{Fano} using equation 5.1 were performed as in chapter 4 for the same four materials (beryllium, graphite (1.7 g/cm^3), aluminum, copper), three incident mono-energetic photon beams (50 keV, 300 keV, 1.25 MeV), two incident photon spectra (^{60}Co and 120 kVp tungsten target), three transport cutoffs (1, 3, 10 keV), and seven cavity sizes, or heights (0.1 mm – 10 mm). Except where noted, Monte Carlo transport parameters and other simulation settings were kept consistent across all user codes.^{95,102}

5.2.2 Formalism terms

The largest contributor to the formalism dose to air in equation 5.1 comes from the differential fluence of charged particles ($\Phi_{wall}(E)$) as particles slow down and deposit energy in media and air. The product of fluence and restricted mass collisional stopping powers $\left(\left(\frac{L_{\epsilon}(E)}{\rho}\right)_{air} \text{ and } \left(\frac{L_{\epsilon}(E)}{\rho}\right)_{wall}\right)$ were calculated using a modified version of the **FLURZnrc** code. The modified code scored the quantity $\Phi_{wall}\left(\frac{L}{\rho}\right)_i$, where i is air or wall material, for each charged particle step, binning the result in a histogram with bins of equal logarithm width in charged particle energy. Like the **cavity** dose calculations done in chapter 4, *Fano* conditions were implemented which discarded scattered photons after interactions and regenerated their original direction and en-

ergy.

The same modified **FLURZnrc** code was used to calculate the spectra of initial energies of charged particles set in motion as photoelectrons, Compton scattering processes, and pair production in media and air ($S_{wall}(E)$ and $S_{air}(E)$). Spectra were finely organized into 1000 bins, uniformly sized in log-space, from the lowest charged particle creation cutoff ($AE = ECUT$) to the maximum photon energy, and a large number of histories were simulated to reduce statistical uncertainties. The track-end terms in the second line of equation 5.1 were calculated using **SPRRZnrc** and are the same track-end doses used in the Spencer-Attix formalism. These are charged particles which cross the lowest threshold (energy ϵ) during particle transport $\left(\epsilon \Phi_{wall}(\epsilon) \left(\frac{L_{\epsilon}(\epsilon)}{\rho} \right)_{wall} \right)$ and are considered to be deposited locally, as well as charged particles which are created below ϵ , $\left(\int_0^{\epsilon} dE S_{wall}(E) E \right)$.

The energy deposition, $\chi(E)$, seen in the third line of equation 5.1, was calculated in the **EGSnrc cavity** user code.⁹⁵ This chamber-specific and energy-dependent quantity was calculated using a source of mono-energetic electrons distributed evenly throughout the cavity volume. A source electron with an initial energy was initiated with a random position and direction vector in the cavity, and the energy deposited in the cavity was scored. $\chi(E)$ represents the average dose per electron deposited over many independent histories. Python's NumPy¹⁰³ and SciPy¹⁰⁴ libraries were used to take the derivative of $\chi(E)$ with respect to energy, which appears as $\chi'(E)$ in the first line of equation 5.1. Linear interpolation and integration were also handled with NumPy and SciPy. All material densities, masses, and Z/A ratios used were internal to **EGSnrc** for consistency across calculations. The sum of the formalism parameters was divided by the **FLURZnrc** calculated collision kerma to derive dose ratios analogous to those presented in chapter 4. One variance reduction technique

was used in both the **FLURZnrc** and **SPRRZnrc** codes: *photon forcing = on* with one interaction forced in the wall.

5.2.3 Spencer-Attix cavity theory calculations

Monte Carlo calculations of the Spencer-Attix cavity theory requires a transport cutoff of charged particles equal to the average threshold energy necessary to cross the chamber cavity. The most common method is to match the mean chord length of the chamber, which was described in section 1.2.3, to the CSDA range of charged particles with energies matching the low energy transport cutoff (Δ). The utility of the novel formalism will depend on its ability to outperform dose ratios predicted by Spencer-Attix. No additional calculations will be required to generate Spencer-Attix dose ratios as the same data used in the calculation of D_{air}^{Fano} in equation 5.1 can be used in calculations for the Spencer-Attix formalism.

5.3 Results

5.3.1 Calculation of cavity theory formalism inputs

Dose spectra

The dose spectra calculated by **FLURZnrc**, due to charged particles set in motion and slowing down in uniform wall media are shown in figures 5.1 and 5.2. These are used in the first term of the formalism and are responsible for the majority of the dose in an air-filled cavity at high energies. The differences in photon interaction cross-sections between materials contributes to the difference in dose spectra at 1.25 MeV, where Compton interactions are dominant. At lower incident energies small

Figure 5.1: Differential dose spectra of charged particles in the 10 mm cavity height of three chamber wall materials from a 1.25 MeV photon beam with a charged particle transport cut-off of 1 keV.

photoelectric peaks can be distinguished, especially in the higher-Z copper wall media as the cross-section for this increases relative to Compton scattering. Dose spectra in air are calculated at the same time as for wall media, using wall media charged particle transport and multiplying the energy deposited at each condensed history step by the ratio of mass-restricted stopping powers for air and wall, evaluated at the mid-point between the initial and final kinetic energies of the step, $\left(\frac{L_\epsilon(E)}{\rho}\right)_{\text{wall}}^{\text{air}}$.

Figure 5.2: Differential dose spectra comparing graphite (Gr) and copper (Cu) walled chambers for three incident energies, 1 keV transport cutoff.

Initial charged particle spectra

FLURZnrc calculations of the initial charged particle spectra set in motion in uniform wall media are shown in figures 5.3 and 5.4. These are used in the third line of equation 5.1, in part, to calculate the dose due to differences in scattering probabilities between the wall medium and air. The photopeaks and Compton scattering distributions are easily distinguishable in the lower incident energy plots.

Figure 5.3: Initial charged particle spectra in three homogeneous materials for a 1.25 keV incident photon beam and a charged particle creation cutoff of $\text{ECUT} = 1 \text{ keV}$.

Figure 5.4: Initial charged particle spectra in copper for three photon beam energies and a charged particle creation cutoff of $\text{ECUT} = 1 \text{ keV}$.

Energy deposition spectra

Energy deposition spectra calculated using the **cavity** user-code are shown in figure 5.5. These curves represent the average amount of energy (MeV/g) deposited in the chamber cavity by a source of mono-energetic electrons distributed randomly, and with a random direction, throughout the cavity. Energy deposition depends heavily on electron energy and cavity size, with maximum deposition occurring near the low energy range of the spectra. This quantity is calculated for the third term in the formalism as part of the dose due to differences in scattering probabilities between the wall medium and air. Figure 5.5 shows the effect of material specific electron backscatter properties which slightly increases the dose deposited in cavities with increasing atomic number (Z). The derivative of $\chi(E)$ with respect to energy, $\chi'(E)$, modifies the relative contributions to dose to the cavity from the wall and air in the first term of equation 5.1.

Another way to understand this quantity is to divide the energy deposited by the initial energy of the electron. This fractional energy deposition is seen in figure 5.6 and underlines the fact that low energy electrons deposit dose locally. Only 5% of the energy of a 100 keV electron will be deposited in a large, 10 mm high, cavity, but 90% of the energy of a 10 keV electron will be deposited in the same cavity size. In 1971 L. V. Spencer published “Remarks on the Theory of Energy Deposition in Cavities” that shows a similar figure to figure 5.6.¹⁸ Overlaid on the fractional energy deposition curves is his Spencer-Attix theory Δ approximation and an acknowledgement that once the methods for calculating such curves were available, they were worth incorporating.

Figure 5.5: Energy deposition functions for three chamber wall media with varying air cavity sizes. Curves represent the average energy deposited in the cavities by electrons as a function of initial electron kinetic energy, E .

Figure 5.6: Fractional energy deposition in three chamber wall media with varying air cavity sizes. Curves represent the fraction of energy deposited by electrons in the cavities as a function of initial electron kinetic energy, E .

5.3.2 Dose ratios

Formalism dose ratios

Values of D_{air}^{Fano} (and D_{wall}^{Fano}) can be calculated using equation 5.1 with the quantities presented in section 5.3.1. The dose-to-wall, D_{wall}^{Fano} , is given by

$$D_{wall}^{Fano} = \int_{\epsilon}^{E_0} dE \Phi_{wall}(E) \left(\frac{L_{\epsilon}(E)}{\rho} \right)_{wall} + \epsilon \Phi_{wall}(\epsilon) \left(\frac{L_{\epsilon}(\epsilon)}{\rho} \right)_{wall} + \int_0^{\epsilon} dE S_{wall}(E) E. \quad (5.2)$$

where ϵ is the transport cutoff energy for creating and tracking charged particles, E_0 is the maximum incident photon energy, $\Phi_{wall}(E)$ is the charged particle slowing down spectra in the medium including secondary “knock-on” electrons liberated by charged particle collisional interactions, $\left(\frac{L_{\epsilon}(E)}{\rho} \right)_{wall}$ is the restricted mass collisional stopping power in the wall material, and $S_{wall}(E)$ is the initial charged particle spectra by the incident source. The second and third terms of equation 5.2 are the track-end contributions to dose from charged particles crossing the transport cutoff (ϵ) and from charged particles created below the transport cutoff, respectively. Values of the ratio $D_{air}^{Fano} / D_{wall}^{Fano}$ can then be compared to direct Monte Carlo calculated values of the same quantity presented in chapter 4.

For a 1.25 MeV mono-energetic incident photon energy and a transport cutoff of 1 keV, formalism dose ratios differ by less than 0.13% over all cavity sizes and all materials compared to direct Monte Carlo calculated **CAVRZnrc** ratios. For the 300 keV mono-energetic incident energy, 1 keV transport cutoff, the formalism dose ratios differ by less than 0.67% from **CAVRZnrc** and for the 50 keV mono-energetic incident energy the formalism dose ratios differ by less than 5.29%. Dose ratio results for an incident cobalt-60 spectra (Mora 10x10 spectra distributed with **EGSnrc**)¹⁰⁵ show similar percent differences to the 1.25 MeV results in the graphite

and copper walled chambers compared for 1 keV transport cutoffs while the 120 kVp tungsten xray target showed similar percent differences to the 50 keV results. These are summarized in tables 5.1 and 5.2.

Table 5.1: Maximum percent difference in dose ratio between formalism and direct Monte Carlo **CAVRZnrc** calculated dose ratios over all seven cavity heights investigated (0.1 to 10 mm) with $\epsilon = 1$ keV transport cutoffs. The 120 kVp entry is a tungsten x-ray target spectra and the ^{60}Co spectra is from Mora *et al.*¹⁰⁵ Dashes (—) imply that no calculations were performed.

Maximum percent difference for incident photon beams of energy:					
Wall media	120 kVp	0.05 (MeV)	0.30 (MeV)	^{60}Co	1.25 (MeV)
Beryllium	—	-5.23	-0.57	—	-0.10
Graphite	-1.63	-1.68	-0.22	-0.10	-0.05
Aluminum	—	0.81	0.28	—	-0.09
Copper	6.40	5.29	0.67	0.19	0.13

Table 5.2: Mean percent difference in dose ratio between formalism and direct Monte Carlo **CAVRZnrc** calculated dose ratios over all seven cavity heights investigated (0.1 to 10 mm) with $\epsilon = 1$ keV transport cutoffs. The 120 kVp entry is a tungsten x-ray target spectra and the ^{60}Co spectra is from Mora *et al.*¹⁰⁵

Mean percent difference for incident photon beams of energy:					
Wall media	120 kVp	0.05 (MeV)	0.30 (MeV)	^{60}Co	1.25 (MeV)
Beryllium	—	-3.54	-0.32	—	-0.01
Graphite	-1.42	-1.34	-0.15	-0.03	-0.02
Aluminum	—	0.54	0.09	—	-0.02
Copper	4.62	4.06	0.51	0.13	0.05

Figure 5.7 shows the ratio of D_{air}^{Fano} to D_{wall}^{Fano} (given by equations 5.1 and 5.2, respectively) due to a 1.25 MeV mono-energetic photon beam incident on plane-parallel pancake ion chambers with graphite, beryllium, aluminum, and copper walls. Solid lines show values predicted by the formalism while dotted lines represent results of direct Monte Carlo calculations with **CAVRZnrc**. Results for ^{60}Co , 300 keV mono-energetic, and 50 keV mono-energetic beams are shown in figures 5.8–5.10.

Figure 5.7: Chamber cavity dose ratios under *Fano* conditions predicted by the cavity theory formalism (solid lines) compared with direct Monte Carlo calculations with **CAVRZnrc** (dotted lines and square data points) for a 1.25 MeV mono-energetic plane-parallel photon beam incident on a pancake ion chamber made with beryllium, graphite, aluminum, and copper walls as a function of cavity height. All results correspond to a low energy threshold for charged particle creation and transport ($\epsilon = \text{AE} = \text{ECUT} = 1 \text{ keV}$).

Figure 5.8: Chamber cavity dose ratios under *Fano* conditions predicted by the cavity theory formalism (solid lines) compared with direct Monte Carlo calculations with **CAVRZnrc** (dotted lines and square data points) for a ^{60}Co plane-parallel photon beam incident on a pancake ion chamber made with copper walls as a function of cavity height. All results correspond to a low energy threshold for charged particle creation and transport ($\epsilon = \text{AE} = \text{ECUT} = 1 \text{ keV}$).

Figure 5.9: Chamber cavity dose ratios under *Fano* conditions predicted by the cavity theory formalism (solid lines) compared with direct Monte Carlo calculations with **CAVRZnrc** (dotted lines and square data points) for a 0.3 MeV mono-energetic plane-parallel photon beam incident on a pancake ion chamber made with beryllium, graphite, aluminum, and copper walls as a function of cavity height. All results correspond to a low energy threshold for charged particle creation and transport ($\epsilon = \text{AE} = \text{ECUT} = 1 \text{ keV}$).

Figure 5.10: Chamber cavity dose ratios under *Fano* conditions predicted by the cavity theory formalism (solid lines) compared with direct Monte Carlo calculations with **CAVRZnrc** (dotted lines and square data points) for a 0.05 MeV mono-energetic plane-parallel photon beam incident on a pancake ion chamber made with beryllium, graphite, aluminum, and copper walls as a function of cavity height. All results correspond to a low energy threshold for charged particle creation and transport ($\epsilon = AE = ECUT = 1$ keV).

Results for larger transport cutoffs, $AE = ECUT = \epsilon = 3$ and 10 keV, had generally larger percent differences than in 1 keV comparisons, but still tracked the trend of dose ratios over all cavity heights. Unlike Spencer-Attix theory, which requires a transport cutoff equal to the energy required by a charged particle to cross the chamber cavity (10 keV in many practical chambers), this highlights the need to track charged particles to the lowest possible energies in all situations when calculating dose ratios for the novel theory. Figures 5.11–5.13 show formalism dose ratios calculated with low energy thresholds for charged particle creation and transport ($\epsilon = AE = ECUT$) equal to 1, 3, and 10 keV for two high-Z wall materials (copper and aluminum) and two incident energies (1.25 MeV and 300 keV).

Figure 5.11: Values of $D_{air}^{Fano} / D_{wall}^{Fano}$ as a function of chamber cavity height for a 1.25 MeV mono-energetic plane-parallel photon beam incident on an air-filled pancake chamber with copper walls, predicted using the cavity theory given by equation 5.1 (solid line) and direct Monte Carlo calculations with **CAVRZnrc** (dotted line, squares) under *Fano* conditions. Results are shown for a low energy threshold for production and transport of charged particles of ($AE = ECUT = \epsilon = 1, 3$, and 10 keV).

Figure 5.12: Values of $D_{air}^{Fano} / D_{wall}^{Fano}$ as a function of chamber cavity height for a 1.25 MeV mono-energetic plane-parallel photon beam incident on an air-filled pancake chamber with aluminum walls, predicted using the cavity theory given by equation 5.1 (solid line) and direct Monte Carlo calculations with **CAVRZnrc** (dotted line, data points) under *Fano* conditions. Results are shown for a low energy threshold for production and transport of charged particles of ($AE = ECUT = \epsilon = 1, 3$, and 10 keV).

Figure 5.13: Values of $D_{air}^{Fano} / D_{wall}^{Fano}$ as a function of chamber cavity height for a 0.3 MeV mono-energetic plane-parallel photon beam incident on an air-filled pancake chamber with aluminum walls, predicted using the cavity theory given by equation 5.1 (solid line) and direct Monte Carlo calculations with **CAVRZnrc** (dotted line, data points) under *Fano* conditions. Results are shown for a low energy threshold for production and transport of charged particles of (AE = ECUT = ϵ = 1, 3, and 10 keV).

Spencer-Attix dose ratios

Using available data computed for the formalism values, two Spencer-Attix theory comparisons were made in each energy and material combination with direct Monte Carlo calculated dose ratios for cavity heights of 0.15 mm ($\Delta = \text{AE} = \text{ECUT} = 3$ keV) and 1.39 mm ($\Delta = \text{AE} = \text{ECUT} = 10$ keV). Table 5.3 shows the results of this investigation. Spencer-Attix cavity theory predicts dose ratios very well for 1.25 MeV photon beams incident on chambers with similar effective atomic numbers to air, but poorly, in general, for low energy photon beams. Table 5.4 tabulates the full comparison between Spencer-Attix and direct Monte Carlo calculated dose ratios and novel formalism and direct Monte Carlo calculated dose ratios. A value of 1 indicates very good agreement between cavity theory and direct Monte Carlo calculations.

Table 5.3: Percent difference between Spencer-Attix dose ratios compared to direct Monte Carlo calculated dose ratios using **CAVRZnrc** for two Δ values (3 and 10 keV) corresponding to cavity heights of 0.15 and 1.39 mm in four cavity chamber wall materials and three incident photon beams.

Energy (MeV)	Percent difference (%) between Spencer-Attix dose ratios and direct Monte Carlo calculated dose ratios							
	Beryllium		Graphite		Aluminum		Copper	
	0.15	1.39	0.15	1.39	0.15	1.39	0.15	1.39
0.05	-8.6	-14.6	-3.2	-6.2	3.6	8.0	8.2	20.6
0.3	-0.2	-0.5	-0.1	-0.2	0.2	0.4	1.2	1.7
1.25	-0.01	0.02	-0.03	-0.03	0.1	-0.03	0.6	0.2

Table 5.4: Comparing the novel formalism (using $\epsilon = 1$ keV) and Spencer-Attix to direct Monte Carlo calculated dose ratios using **CAVRZnrc** in two chamber cavity heights (0.15 and 1.39 mm, corresponding to $\Delta = 3$ and 10 keV) with varying incident energy and wall materials $\left(\frac{Dose\ ratio\ novel}{Dose\ ratio\ direct}\right)$ and $\left(\frac{Dose\ ratio\ SA}{Dose\ ratio\ direct}\right)$.

0.15 mm cavity height	0.05 MeV			Cu	0.3 MeV			Cu	1.25 MeV			Cu
	Be	Gr	Al		Be	Gr	Al		Be	Gr	Al	
Spencer-Attix	0.917	0.969	1.037	1.085	0.998	0.999	1.002	1.012	1.000	1.000	1.001	1.006
Novel	0.951	0.983	1.004	1.033	0.999	0.999	0.999	1.004	1.000	1.000	1.000	1.001
1.39 mm cavity height	0.05 MeV			Cu	0.3 MeV			Cu	1.25 MeV			Cu
	Be	Gr	Al		Be	Gr	Al		Be	Gr	Al	
Spencer-Attix	0.864	0.940	1.084	1.230	0.995	0.998	1.004	1.018	1.000	1.000	1.000	1.002
Novel	0.967	0.987	1.005	1.040	0.996	0.998	1.001	1.006	1.000	1.000	1.000	1.000

Comparing the novel formalism dose ratios to Spencer-Attix dose ratios, the novel cavity theory (using the most accurate transport cutoff, $\epsilon = 1$ keV) was much better at predicting the correct dose in every situation except for in high energy (1.25 MeV), similar radiological materials to air (beryllium and graphite), where the predictions were equal. Tables 5.5 and 5.6 show summary comparisons between the Spencer-Attix and novel theory at the two sample Δ values (corresponding to cavity heights of 0.15 and 1.39 mm), comparing the ratio of percent differences of each theory with direct Monte Carlo calculated dose ratios. The tables, along with figures 5.14 and 5.15, which are similar to figures 5.11 and 5.10 with the addition of Spencer-Attix calculated dose ratios, respectively, highlight the ability of the novel formalism to track the trend of dose ratios through the full range of cavity heights investigated. The increased accuracy of the formalism over Spencer-Attix is on average two to six times better, when grouped by incident energy, and two to four times more accurate for graphite walled ion chambers.

Table 5.5: Ratio of percent differences when compared to direct Monte Carlo calculated dose ratios $\frac{\%_{Spencer-Attix}}{\%_{novel}}$ for two sample Δ values (3 and 10 keV, corresponding to cavity heights of 0.15 and 1.39 mm). The values demonstrate how many times more accurate the novel formalism is compared to Spencer-Attix as a function of incident photon beam energy.

Cavity height	0.05 (MeV)	0.30 (MeV)	1.25 (MeV)	All combined
0.15 mm	2.3	2.5	6.3	2.3
1.39 mm	5.4	2.3	3.6	5.0

Table 5.6: Ratio of percent differences when compared to direct Monte Carlo calculated dose ratios $\frac{\%_{Spencer-Attix}}{\%_{novel}}$ for two sample Δ values (3 and 10 keV, corresponding to cavity heights of 0.15 and 1.39 mm). The values demonstrate how many times more accurate the novel formalism is compared to Spencer-Attix as a function of cavity chamber wall material.

Cavity height	Beryllium	Graphite	Aluminum	Copper
0.15 mm	1.7	1.9	8.1	2.7
1.39 mm	4.0	4.3	12.3	4.9

Figure 5.14: Similar to figure 5.11, values of $D_{air}^{Fano} / D_{wall}^{Fano}$ as a function of chamber cavity height for a 1.25 MeV mono-energetic plane-parallel photon beam incident on an air-filled pancake chamber with copper walls, predicted using the cavity theory given by equation 5.1 (solid line), Spencer-Attix cavity theory (triangles), using the same underlying data used in equation 5.1, and direct Monte Carlo calculations with **CAVRZnrc** (dotted line, squares) under *Fano* conditions. Results are shown for a low energy threshold for production and transport of charged particles of ($AE = ECUT = \epsilon = 1, 3$, and 10 keV). Spencer-Attix dose ratios are evaluated for cavity sizes of 0.15 and 1.39 mm corresponding to ($\Delta = 3$ and 10 keV).

Figure 5.15: Similar to figure 5.10, chamber cavity dose ratios under *Fano* conditions are predicted by the cavity theory formalism (solid lines) compared with Spencer-Attix cavity theory predictions (triangles), using the same underlying data used for results given by equation 5.1, compared with direct Monte Carlo calculations with **CAVRZnrc** (dotted lines, squares) for a 0.05 MeV mono-energetic plane-parallel photon beam incident on a pancake ion chamber made with graphite, aluminum, and copper walls as a function of cavity height. Novel formalism and **CAVRZnrc** results correspond to a low energy threshold for charged particle creation and transport ($\epsilon = \text{AE} = \text{ECUT} = 1 \text{ keV}$) while Spencer-Attix dose ratios are evaluated for cavity sizes of 0.15 and 1.39 mm corresponding to ($\Delta = 3$ and 10 keV).

5.4 Summary

Monte Carlo calculations of charged particle slowing-down dose spectra, initial energies of charged particles set in motion ($S_{air}(E)$ and $S_{wall}(E)$), energy deposition in the air cavity of an ion chamber free-in-air ($\chi(E)$), and dose to the uniform wall material ($K_{collision, wall}$) were performed using the **FLURZnrc**, **SPRRZnrc**, and **cavity EGSnrc** user-codes. These were used as inputs to the novel cavity theory formalism given by equation 5.1 to determine dose ratios over a large range of clinically relevant energies and material configurations. Formalism dose ratios were compared to Spencer-Attix dose ratios and compared to direct Monte Carlo calculated values over all cavity sizes and material combinations investigated.

The terms calculated here for equation 5.1 were introduced in chapter 2. Notably, the dependencies of each input term are discussed in section 2.6. As a brief review, the dose spectra is the product of the source-dependent, unperturbed fluence of charged particles in the medium and the mass-restricted stopping powers of the medium and cavity $\left[\Phi(E), \left(\frac{L_e(E)}{\rho} \right)_{air} \text{ and } \left(\frac{L_e(E)}{\rho} \right)_{wall} \right]$. The dose spectra depends only on the properties of the source of ionizing radiation and on the material properties of the ion chamber. For chambers that have walls with atomic numbers (Z) lower than the cavity material, in this case air, the dose ratios increase with increasing cavity size. Conversely, for chambers that have walls with higher-Z walls than the cavity material, in this case air, the dose ratios decrease with increasing cavity size. Calculations of this type generally take a few seconds to minutes to achieve sub-0.05% statistical uncertainties.

The spectra of initial energies of charged particles in the air cavity [$S_{air}(E)$] and wall material [$S_{wall}(E)$] depend only on the properties of the source of ionizing radiation and on the material properties of the ion chamber. Compton scattering dominates

the spectra at higher energies and both Compton scattering and liberated photoelectrons contribute to the spectra at lower incident energies. Calculations of this type are very fast, taking only a few seconds to minutes to achieve sub-0.05% statistical uncertainties.

As stated previously, energy deposition spectra ($\chi(E)$), which Spencer would have liked to employ in his original cavity theory formulation,¹⁸ depends only on the details of the detector - in this case an ion chamber - including the cavity size and wall material. This quantity is decoupled from the incident external source and corresponding dose spectrum it yields in a solid slab of wall material under Fano conditions (*i.e.* using the photon regeneration Monte Carlo technique discussed in section 3.2.2 that removes attenuation and scatter). As demonstrated in figure 5.5, the size of the cavity is the primary factor in how much energy a given electron will deposit. A much smaller dependency is the type of wall material surrounding the cavity. Higher-Z materials will backscatter a larger portion of charged particles back into the cavity than lower-Z materials, resulting in a higher fraction of initial kinetic energy deposited. Calculations of $\chi(E)$ are also very fast, taking minutes to achieve small statistical uncertainties over the full energy range. Additionally, as this quantity depends only on the details of a given detector, calculations need only be done once over the full range of energies required, and the $\chi(E)$ function can be applied to other sources incident on that detector. The derivative of $\chi(E)$ with respect to energy, $\chi'(E)$, was a simple and robust computation using the Python library SciPy.

Using the parameters discussed above, novel formalism dose ratios of D_{air}^{Fano} and D_{wall}^{Fano} were calculated from equations 5.1 and 5.2. These were compared to direct Monte Carlo dose ratios calculated by **CAVRZnrc**, agreeing well with those benchmark values, and tracked the trend of dose ratios as a function of cavity height. Using

available data, Spencer-Attix cavity theory dose ratios were also calculated and compared to the same direct Monte Carlo calculated dose ratios. Spencer-Attix cavity theory predicted dose ratios as expected, with good agreement at high energy and in radiologically similar wall materials to air, but poor agreement at lower incident energies and for radiologically dissimilar wall materials. Novel formalism dose ratios were compared to Spencer-Attix generated dose ratios and the novel formalism was much more accurate over a wide range of clinically relevant energies and chamber wall materials.

Like Spencer-Attix cavity theory, the novel formalism in equation 5.1 may be applied to in-phantom measurements as long as attenuation, scatter, and the divergence of the source $[S(E, \vec{\Omega}, \vec{x})]$ are accounted for. Unlike Spencer-Attix and other historical theories,^{10,21} the novel formalism does not rely on ambiguously chosen parameters or concepts. There are no cavity size, material composition, or incident beam energy-dependent factors, like Δ ,^{20,22,25,26} nor do the well known Bragg-Gray conditions (section 1.2.2) need to be applied for accurate predictions.

The analogous quantity to Δ in the novel formalism, ϵ , is chosen so that charged particle range and bremsstrahlung production are negligible, which leads to choosing the smallest and most accurate value possible. This removes the ambiguous choice involving which value of Δ to use and eliminates the computational burden of calculating detour factors, as introduced in section 1.2.3.²⁰ Cavity size-dependence and charged particle fluence perturbations by the cavity are explicitly addressed in the derivation of D_{air}^{Fano} through a perturbation fluence $[\Phi_p(E)]$, which is born out in the energy deposition function, $\chi(E)$. Additionally, the liberation of charged particles in the cavity, which violates the second Bragg-Gray cavity condition, are permitted and allow this novel cavity theory to be applied over a much wider range of cavity sizes,

cavity wall materials, and incident beam energies than ever before.

Chapter 6

Conclusions

6.1 Overview

Radiation dosimetry has historically relied on cavity theory to determine the dose to a medium from the measured dose to the cavity volume of a detector at a point of measurement. The mathematical expressions describing the particle interactions that contribute to dose deposition are intractable, and led early scientists to make limiting assumptions that allow for analytical expressions for dose deposition that can be easily described. The assumptions involved, however, imposed limitations on physical situations over which these cavity theories could be applied.

Two separate avenues have been taken to address the limitations of cavity theory in making generally accurate predictions:

1. introducing correction factors calculated using Monte Carlo methods, and
2. restricting the range of physical conditions where the use of cavity theory can be applied.

The introduction of correction factors has expanded the general range of cavity theory

accuracy, but not enough to discourage a transition to direct Monte Carlo calculations as the basis for dose determination in modern dosimetry protocols. As cavity theory is the only direct means we have for obtaining a physical intuition for how detector measurements relate to dose, it is very important to develop a cavity theory that can be generally applied, serve as a useful “second check,” and provide a link to our understanding of the underlying physical processes.

The novel cavity theory presented in this thesis addresses many of the limiting assumptions that prohibited previous theories from general accuracy and application. Most notably, the longstanding conditional requirements of Bragg-Gray cavity theory on fluence perturbations and cavity charged particle liberation are lifted by the derivation and implementation of a perturbation fluence. Additionally, all ambiguity regarding cavity size-dependent choices are removed with direct Monte Carlo calculation of primary data. This approach comes with added complexity, but the reward is both worthwhile and advantageous in regards to general applicability and accuracy.

6.2 Summary and conclusions

In chapter 2 a generalized cavity theory formalism and associated stopping power ratio have been derived from the Boltzmann transport equation for charged particles produced by a broad, parallel, unattenuated, unscattered external source of photons. Its application relies on quantities accessible through routine Monte Carlo simulations under a consistent set of interaction cross-sections, stopping powers, and scattering powers. Convergence with the Spencer-Attix theory has been shown in the small cavity limit, and when the cavity material and surrounding medium are radiologically equivalent (section 2.5.1), where Spencer-Attix is known to be an accurate predictor of dose. In the large cavity limit, where the dimensions of the cavity are comparable

to the range of charged particles crossing it, the stopping-power ratio converges, as expected, to the ratio of mass energy absorption coefficients (section 2.5.2).

Analogous to the Spencer-Attix stopping-power ratio, the formalism presented here depends upon a low-energy cut-off ϵ below which it is assumed that charged particles at or below this energy are deposited locally. However, unlike the Spencer-Attix formalism, this low-energy cut-off is chosen independently of cavity size, subject to other constraints imposed by assumptions made in the derivation (section 2.6). Changes in detector response with cavity dimensions are accounted for via a charged particle energy deposition function, $\chi(E)$. Conveniently, $\chi(E)$ depends only on the cavity dimensions and on the material of the surrounding medium, and not the incident source. Therefore, calculations do not need to be repeated for a chamber when it is used in a different physical situation.

The formulation of the generalized cavity theory and associated stopping power ratio, denoted here as $\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air}$, lends itself to broad applicability in terms of the size of cavities, chamber materials, and incident beam energies. In principle, there are no restrictions on cavity size or chamber wall/cavity material combinations and, specifically, no requirement that Bragg-Gray conditions be met. Furthermore, like the Spencer-Attix and Bragg-Gray formalisms, $\left(\frac{\bar{L}_\epsilon}{\rho}\right)_{wall}^{air}$ ratios are likewise applicable to phantom dosimetry and other situations that consider attenuation and scatter of the source, and where the fluence of charged particles in the medium of interest varies with depth.

In chapter 3 the Monte Carlo method and **EGSnrc**'s software user-codes used throughout this work were presented. Details regarding the physical processes simulated, and the software simulation parameters, to calculate dose to ion chamber cavities were introduced. In chapter 4, direct Monte Carlo calculations of ion cham-

ber cavity dose ratios were presented. These dose ratios investigated the effect of Monte Carlo transport parameter choice and created a library of dose ratios which are considered to be an accurate reflection of the ratio of doses absorbed in the chamber cavity filled with air to a cavity filled with uniform wall material. Consistency was ensured by employing multiple methods of dose scoring using independent Monte Carlo user-code packages. As a side note, this investigation showed that cavity chamber dose calculations are especially sensitive to changes in two transport parameters at low incident energies. These types of calculations must simulate atomic relaxations and photoelectron angular sampling to ensure accuracy.

In chapter 5 the calculation of individual inputs to the novel formalism were introduced and completed. As mentioned previously, the calculation of these quantities using the smallest transport parameters removes all ambiguity regarding cavity size fluence corrections and low energy transport thresholds that are encountered when using other cavity theory formalisms. The total time to complete Monte Carlo calculations for the novel formalism ranged between minutes to at most a half hour, while direct calculations of cavity dose in **CAVRZnrc** ranged between one to seventeen hours. While the computational overhead and setup time for the novel formalism is much longer than for direct Monte Carlo chamber dose calculations, the ten to thirty times improvement in computational efficiency over direct, analog Monte Carlo calculations, is advantageous in many situations, as accuracy is generally preserved. Spencer-Attix cavity theory predictions of dose ratios were conducted using the common available data, and comparisons between the novel formalism, Spencer-Attix, and the direct Monte Carlo calculated dose ratios were made. The new formalism predicts dose ratios far more accurately than all cavity theories known by this author to date over the broad range of energies and materials shown here.

6.3 Future work

There are a number of dosimetry protocols published for various applications. At higher incident energy, ^{60}Co to 50 MV, photon beams there are the TG-51^{4,5} and TRS-398¹⁰⁶ protocols, for ‘orthovoltage,’ below 300 kV, xray beams there are the TG-61^{6,7} and TRS-277¹⁰⁷ protocols, and for small and non-standard fields there is the work done by Alfonso *et. al.*¹⁰⁸ Some of these dosimetry protocols historically had a foundation in Spencer-Attix cavity theory,⁴ but recent updates⁵ have calculated kQ factors exclusively by Monte Carlo methods with no connection to cavity theory. The lower energy dosimetry protocols do not use cavity theory.^{6,7}

The fractured nature of dosimetry speaks to the difficulty of deriving a unified cavity theory that is applicable over the full range of clinical situations. With current dosimetry protocols using pre-calculated kQ values, users must wait for published values for new detectors. There is the potential for the formalism presented here to fill a valuable role as a user accessible confirmation tool that has its foundation in the physics of cavity theory.

One can speculate that the cavity theory formalism presented in this work may be able open the market for detectors with non-air-equivalent wall materials which have been previously impractical due to their large correction factors involved with their use. It could also possibly allow manufacturers to shrink detector sizes, barring any measurement uncertainties, to overcome the problem of a lack of lateral charged particle equilibrium in narrow treatment beams that poses a challenge with current ion chambers.

Another known issue for vented ionization chambers are the signal variations observed when exposed to large changes in environmental conditions, including temperature and atmospheric pressure.^{79,101} This novel formalism may account for these ob-

served variations, that are not accounted for using the standard temperature-pressure correction, which are important for establishing accurate radiation dose calibrations in regions of high altitude (*e.g.* Calgary and Mexico City). It has been shown that the usual methods of correcting for large deviations in pressure from reference calibration conditions are inaccurate by several percent depending on the chamber and radiation beam energy. When it concerns radiation therapy, such large deviations are unacceptable.

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