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GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

GRASP: A PROGRAM TO CALCULATE SOME GAMMA SHIELDING PARAMETERS

MSc THESIS

Issa KARNIK

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Thesis Advisor: Prof. Dr. Mehmet BEKTAŞOĞLU

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The thesis work titled "GRASP: A PROGRAM TO CALCULATE SOME GAMMA SHIELDING PARAMETERS" prepared by Issa Karnik was accepted by the following jury on 01/03/2023 by unanimously/majority of votes as a MSc THESIS in Sakarya University Graduate School of Natural and Applied Sciences, Physics department.

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Issa KARNIK

To my mother and my father

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Issa Karnik

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ABBREVIATIONS

GSP : Gamma shielding parameters

MAC : Mass attenuation coefficient

LAC : Linear attenuation coefficient

HVL : Half value layer

TVL : Tenth value layer

MFP : Mean free path

SYMBOLS

Z	: Atomic number
$\mathbf{Z_{eff}}$	: Effective atomic number
E	: Energy [MeV]
w	: Weight fraction
f	: Molar fraction
ρ	: Density [g/cm^3]
μ	: Linear attenuation coefficient [1/cm]
μ_m	**:** Mass attenuation coefficient [cm^2/g]
λ	**:** Mean free path [cm]

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GRASP: A PROGRAM TO CALCULATE SOME GAMMA SHIELDING PARAMETERS

SUMMARY

A new program was developed and tested to calculate a number of gamma-shielding parameters, such as mass attenuation coefficients, linear attenuation coefficients, half value layers, tenth value layers, mean free paths, and effective atomic numbers, for any element, compound, and mixture, in the gamma energy range of 1 keV – 100 GeV. The program is called GRASP, acronym for **G**amma **R**ay **A**ttenuation **S**hielding **P**arameters, it is written with the Python programming language (version 3.9.13) and can function on the Windows operating system. For a given material under study, the program reads the necessary information from a separate input file, where the user defines the composition of the material, the density, and the energy range of interest. Then it looks up cross section values of the elements constituting the material from its database, which is constructed using the XCOM program as a source. The cross-section values of the elements are inserted into built-in equations to calculate the gamma shielding parameters. Tables and graphs are produced and displayed in the output, and options of saving data are given. The results are observed to have great accuracy with theoretical values of mass attenuation coefficients and its derivatives, such as mean free paths and half value layers. Meanwhile for the effective atomic numbers the program is seen to have good accuracy in intermediate energies, a steady overestimation in high energies, and unpredictable uncertainty in the lower energies where absorption edges of elements of high atomic number reside. In comparison to most programs in the literature, GRASP can calculate mass attenuation coefficients at additional energies corresponding to characteristic absorption edges of elements. This gives more definition to its mass attenuation curves. The program is available upon request, it can aid other researchers as a primary or secondary tool to obtain or verify their gamma shielding data.

GRASP: BAZI GAMMA KORUMA PARAMETRELERİNİ HESAPLAYAN BİR PROGRAM

ÖZET

Radyasyon, uzayda veya madde içinde dalgalar ya da parçacıklar şeklinde hareket eden enerjidir. Bir atom veya molekülden bir elektronu uzaklaştırma yeteneğine bağlı olarak radyasyon, *iyonlaştırıcı* ve *iyonlaştırıcı olmayan* şeklinde iki temel gruba ayrılabilir. İyonlaştırıcı olmayan radyasyon (radyo dalgaları, görünür ışık ve mikrodalgalar) atomlardan elektron sökmek için yeterli enerjiye sahip değilken, iyonlaştırıcı radyasyon sahiptir. İyonlaştırıcı radyasyonların oluşturdukları iyonlar DNA'ya zarar verme ve dolaylı olarak kansere neden olma potansiyeli taşırlar. Bu tür radyasyonlar da ayrıca yüklü parçacıklar ve nötr radyasyon olmak üzere iki alt gruba ayrılabilir. Yüklü parçacıklar arasında elektronlar, pozitronlar ve ağır yüklü parçacıklar (protonlar, mezonlar, alfa parçacıkları vb.) yer alır. Nötron ve elektromanyetik radyasyon (örneğin gama ışınları) ise nötr (elektrik yükü olmayan) radyasyon grubundadır. Bu tür radyasyonların madde içine giricilikleri yüklü radyasyonların maddeye nüfuz kabiliyetlerine kıyasla çok daha yüksektir.

Iyonlaştırıcı radyasyonun zararlı etkilerinden korunmak veya bu etkiyi kabul edilebilir seviyelere düşürmek için üç ana yöntem mevcuttur; radyasyon kaynağına olan mesafeyi artırmak, radyasyonun bulunduğu ortamda geçirilen zamanı en aza indirmek ve radyasyonun türüne göre uygun zırhlama yapmak.

Bu tez çalışmasında iyonlaştırıcı mahiyette elektromanyetik radyasyon olan gama ışınlarına odaklanılmıştır. Gamma ışınları yüksek enerjili (~keV/MeV mertebesinde) olup atom çekirdeğinden kaynaklanır. Diğer iyonlaştırıcı radyasyonlar gibi gama ışınının madde ile nasıl etkileştiğini anlamak, ona karşı korunmak ve genel olarak radyasyon maruziyetini kontrol etmek için önemlidir. Bir malzemenin gama ışınlarına karşı zırhlama kabiliyeti gama zırhlama parametrelerinin (*gamma shielding parameters*-GSP) incelenmesiyle anlaşılabilir. Bu parametrelerin arasında *kütle azaltma katsayısı*, *ortalama serbest yol* ve *etkin atom numarası* sayılabilir. Günümüzde gama ışınlarına kaşı zırhlama potansiyeli yüksek malzemelerin geliştirilmesi yönünde yoğun çalışmalar gerçekleştirilmektedir. Birden fazla çeşitte element içeren bileşikler veya birden fazla bileşik içeren karışımlar bu tür malzemeler arasında yer alır. Bu tür malzemeler için gama zırhlama parametrelerinin hesaplanması zaman alabilen, tekrarlanan süreçler olduğu gibi, hesaplayıcının hata yapma ihtimalini de içinde barındırır. Bu nedenle hesaplamaların bir bilgisayardan yararlanılarak yapılması işlem süresini önemli ölçüde kısalttığı gibi hata olasılığını da en aza indirger. Günümüzde yukarıda sözü edilen parametreleri hesaplayabilen çeşitli programlar mevcuttur.

Element, bileşik ve karışımlar için 1 keV – 100 GeV gama enerjisi aralığında kısmi ve toplam azaltma katsayılarını hesaplayan bir foton tesir kesiti veri tabanı olan XCOM 1987 yılında geliştirilmiştir. XCOM'un web tabanlı sürümü 2010 yılından beri erişime açıktır. Kullanıcı, varsayılan enerjilerin yanı sıra 1 keV – 100 GeV enerji aralığındaki herhangi bir enerjiyi manuel olarak ekleyebilir. Bu program kısmı ve toplam kütle

azaltma katsayılarını detaylı olarak hesaplayabilmekle beraber diğer zırhlama parametrelerine dair hesaplama yapmamaktadır.

Auto-Zeff adı verilen bir program önemli gama zırhlama parametrelerinden biri olan etkin atom numaralarını incelemek için geliştirilmiştir. Bu program 10 keV – 1 GeV enerji aralığında foton enerjisinin bir fonksiyonu olarak etkin atom sayılarını hesaplamak için bir enterpolasyon yöntemi kullanmaktadır. Program aynı zamanda tek değerli etkin atom numaralarının hesaplanmasını da sağlar.

Phy-X/PSD, bir dizi gama zırhlama parametresinin hesaplanması için geliştirilmiş çevrimiçi bir yazılımdır. Phy-X aynı anda birden fazla numune için hesaplama yapabilir ve kullanıcıya farklı enerji seçenekleri sunar: XCOM tarafından kullanılan standart enerji aralığı (1 keV – 100 GeV), daha dar aralıktaki (15 keV – 15 MeV) "seçilmiş enerjiler" ve birçok karakteristik X-ışını ve radyoaktif izotop enerjileri.

Literatürde bulunan diğer benzer programlar arasında ParShield, The Rad Toolbox, BXCOM, ve EXABCal sayılabilir. Günümüzde GEANT4, MCNPX ve FLUKA gibi simülasyon programları da birçok araştırmacı tarafından malzemelerin zırhlama parametrelerini incelemek için kullanılmaktadır.

Bu tez çalışması kapsamında malzemelerin kütle azaltma katsayısı, ortalama serbest yol ve etkin atom numarası gibi bir dizi gama zırhlama parametresini 1 keV – 100 GeV foton enerjisi aralığında hesaplayan yeni bir program geliştirilmiş ve test edilmiştir. Gamma Ray Attenuation Shielding Parameters'ın kısaltması olan GRASP isimli bu program Python programlama dilinde (sürüm 3.9.13) yazılmış olup Windows işletim sisteminde çalışabilmektedir. İncelenmekte olan belirli bir malzeme için program, kullanıcının malzemenin bileşimini, yoğunluğunu ve ilgilenilen enerji aralığını tanımladığı ayrı bir girdi dosyasından gerekli bilgileri okur. Daha sonra XCOM programı kullanılarak oluşturulan veri tabanından malzemeyi oluşturan elementlerin kütle azaltma katsayılarına ulaşır. Bu katsayıları gama zırhlama parametrelerini hesaplamak için gerekli denklemlere yerleştirerek tablo ve grafikler üretir. GRASP kullanılarak elde edilen kütle azaltma katsayılarının XCOM'dan elde edilen değerlerle büyük bir uyuma sahip olduğu gözlemlenmiştir. Program, incelenen bileşik ya da karışımda yer alan elementlerin karakteristik soğurma enerjilerine karşılık gelen ek enerjilerde de kütle azaltma katsayılarını söz konusu XCOM değerleriyle genel uyum içinde tahmin edebilmektedir.

Sonuç olarak, bu tez çalışması kapsamında geliştirilen GRASP programı, bazı gama zırhlama parametrelerinin eldesi için diğer mevcut programlara bir alternatif olarak kullanılabilir. Bu tezin hazırlanması aşamasında yalnızca çevrimdışı olarak kullanılabilen program, istenilmesi durumunda diğer araştırmacılarla paylaşılabilir.

1. INTRODUCTION

Radiation is energy that moves through space or material medium in the form of waves or particles. In general, radiation can either be *ionizing* or *non-ionizing*, based on its ability to remove an electron from an atom, or a molecule, in the process called *ionization*. While non-ionizing radiation (for example: radio waves, visible light, and microwaves) does not have enough energy to knock electrons out of atoms, ionizing radiation does, hence, it is more damaging for organisms because the ions it generates have the potential to directly damage DNA and cause cancer [1]. Ionizing radiation can furthermore be divided into two categories: charged particles and neutral radiation. Charged particles include electrons, positrons, and heavy charged particles (protons, mesons, alpha particles, etc.). Neutral radiation includes neutrons and electromagnetic radiation, both of which are not electrically charged, allowing them to penetrate matter more easily than charged particles do. The radiation type of interest for this study is electromagnetic radiation, which includes X rays and gamma rays. The latter in particular is more energetic (~ keV/MeV) and it originates from the nucleus. Understanding how gamma rays interact with matter is important to protect against it, and to control radiation exposure in general.

Researchers study the attenuation behavior of gamma rays through new material mediums to characterize absorber materials and evaluate their performance as shields [2]. The investigated parameters that are linked to shielding against gamma rays are named gamma shielding parameters (GSP), they include mass attenuation coefficients, mean free paths, effective atomic numbers, and many others. Calculation of GSP for composite materials (i.e., materials composed of more than one element), by hand or with regular calculators, is a repetitive and time-consuming process; largely subject to human error. It can be automated with the help of computer programs.

Over the years, many programs have been constructed to calculate one or more GSP. Berger and Hubbell have developed *XCOM* since 1987, a photon cross-section database which calculates partial and total attenuation coefficients for elements, compounds, and mixtures [3]. The 2010 web-based version of XCOM [4] is perhaps the most accessible open-source in the field, with no requirement of registration.

XCOM supports a standard energy grid in the range of 1 keV – 100 GeV, moreover, the user can manually add any energy[1] within that range. Although its database is regarded as the theoretical standard for total attenuation and partial attenuation of elements, XCOM does not provide other GSP, some of which are only a few mathematical operations away. This is where many other programs, including the one at hand, find purpose.

Taylor et al. have created the user-friendly *Auto-Zeff* software [5] for robust calculation of effective atomic numbers (10 keV – 1 GeV). Auto-Zeff uses an interpolation method to calculate effective atomic numbers as a function of photon energy, which is reliable for its agreement with theory and experiment for low Z materials. It also provides the computation of spectra-weighted, single-valued effective atomic numbers.

Şakar et al. have created *Phy-X/PSD* [6], an online software that has been developed for the calculation of a number of GSP. It can also be downloaded as an executable program; however, it requires an academic email to register and gain access to the results, which the program pours into an Excel file. Phy-X can perform calculations for multiple samples at once, and it gives the user different energy options: the standard energy grid used by XCOM (1 keV – 100 GeV), a narrower (15 keV – 15 MeV) labeled as "selected energies", and options for many characteristic X-ray and radioactive isotope energies. But it does not feature the characteristic absorption-edge energies of elements.

Other similar programs available in the literature include *ParShield* [7], *The Rad Toolbox* [8], *BXCOM* [9], and *EXABCal* [10], to name a few. More recently, *Py-MLBUF* [11] is made available, which supports calculations for multi-layered shields as well as single-layered shields. The toolkits of GEANT4 and MCNPX have also been utilized by many researchers to evaluate shielding parameters of materials [12, 13].

In this work, a new program is developed to calculate mass attenuation coefficients, effective atomic numbers, half and tenth value layers, and mean free paths. The name of the program is GRASP, which stands for Gamma Ray Attenuation Shielding Parameters. The code is written with Python, an object oriented, all-purpose

[1] As long as it has a maximum of four significant figures.

programming language. The aim of this thesis is to introduce the program, describe its methods and explore its findings.

2. THEORY

In quantum mechanics, electromagnetic radiation consists of photons. Photons are particles with zero mass, and they travel at the speed of light in a vacuum. The energy of a single photon is directly related to its frequency by the relation

$$E = h\nu \tag{2.1}$$

where E is the energy of the photon, ν is the frequency, and h is the Plank's constant, equals to:

$$h = 6.626 \times 10^{-34}\ \text{J·s} \tag{2.2}$$

or in electron volt units:

$$h = 4.135 \times 10^{-15}\ \text{eV·s} \tag{2.3}$$

The joule (J) is the SI unit for energy. However, in nuclear physics, the convention is to use the electron volt (eV) instead. The electron volt is defined as the kinetic energy gained by an electron accelerating in a potential difference of 1 volt.

$$1\ \text{eV} \cong 1.6 \times 10^{-19}\ \text{J} \tag{2.4}$$

In the electromagnetic spectrum, the section with the shortest wavelengths (highest frequencies) is the ionizing part, because it has the most energy (in the range of keV and MeV). This includes X rays and gamma rays. X rays originate from electron transitions in the orbits of an atom. In one example, when the normal configuration of the orbital electrons of an atom is disrupted by an excitation process, the atom would be in an excited state for a short amount of time. When the atom de-excites and the electrons return to their normal configuration, an X ray is emitted carrying a specific amount of energy, which is equal to the difference of energy between those two orbits. The X ray is then called a *characteristic X ray*.

Gamma rays, in comparison, are more energetic than X rays, and they originate from nuclear sources. When an excited nucleon de-excites (a nucleon transitioning from a higher energy level to a lower energy level), a gamma ray is emitted. These emissions usually follow nuclear reactions or nuclear decay processes, such as beta decays. For

example, the decay scheme of Cs-137 can lead to a population of excited Ba nuclei, which then it de-excites and emits a gamma ray of 0.662 MeV energy (equal to the difference in energy between the initial and final nuclear states of barium) as shown in Figure 2.1.

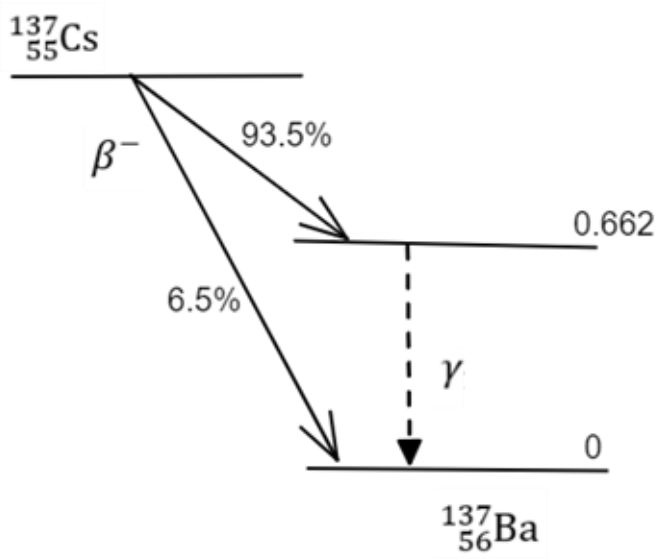

Figure 2.1. Decay scheme of cesium. The beta decay is followed by the emission of a gamma ray 93.5% of the time.

X rays and gamma rays are electrically neutral and do not steadily lose energy as they penetrate matter, like charged particles do. Instead, they can travel some distance before interacting with an atom. When X rays and gamma rays interact, they might disappear and get absorbed or scattered, changing their direction, and losing some of their energy. How far they can travel in a material is a matter of statistics. The probability of interaction per unit distance depends on the energy of the photon, and the specific material it travels through. From an interaction's point of view, there is no real difference between an X ray and a gamma ray, as their energies do overlap. In literature, it is commonplace to only use the term "gamma rays" when describing the interaction of high energy photons with matter. From this point forward, electromagnetic waves of high energy are dubbed as either "gamma rays" or "photons" in this thesis, unless specified otherwise.

2.1. Interaction Mechanisms of Gamma Rays

There are three main mechanisms of energy deposition by gamma rays in matter: the photoelectric effect, the Compton effect, and pair production.

2.1.1. Photoelectric effect

In the photoelectric effect, a photon is absorbed by one of the inner-shell electrons of the atom, the photon completely disappears, and the absorbing electron, called the *photoelectron*, is ejected. A simple illustration of this interaction is shown in Figure 2.2.

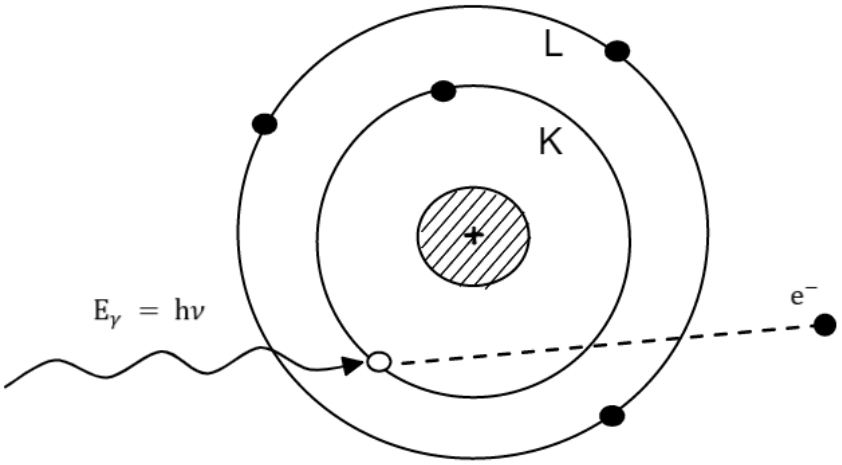

Figure 2.2. A schematic representation of the photoelectric effect. The gamma ray is absorbed by a K-shell electron, and the electron is released.

The photoelectron has a kinetic energy equal to:

$$E_{e^-} = h\nu - E_b \qquad (2.5)$$

where $h\nu$ is the energy of the incident gamma ray, E_{e^-} is the energy of the ejected photoelectron, and E_b represents the binding energy of that same electron in its original shell. This interaction produces an ionized absorber atom with a vacancy in one of its bound shells. This vacancy is quickly filled by one of the electrons from the upper shells. Therefore, one or more characteristic X-ray photons may also be generated.

The photoelectric effect is the dominant interaction process for low gamma ray energies. For absorber materials with a high atomic number Z, the photoelectric probability is also increased. Over all ranges of gamma ray energies and Z, no single

analytic equation is valid for the likelihood of photoelectric absorption per atom [14], although the following reasonable approximation exists:

$$\tau \cong \text{constant} \times \frac{Z^n}{E_\gamma^{3.5}} \tag{2.6}$$

where τ is the photoelectric cross section and has units of m^{-1}. This significant dependency of photoelectric absorption probability on the atomic number of the absorber is the fundamental reason for the prevalence of high-Z materials (such as lead) in gamma-ray shields (see section 2.3.).

2.1.2. Compton effect

Compton effect is the process where a gamma ray interacts with a free or weakly bound electron ($E_\gamma \gg E_b$), and transfers parts of its energy to that electron. A schematic representation of the process is given in Figure 2.3.

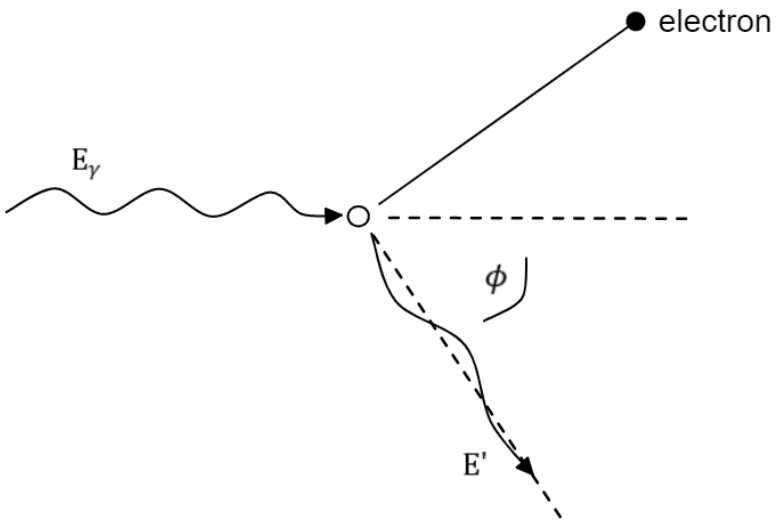

Figure 2.3. Schematic representation of the Compton effect.

This interaction involves the least tightly bound electrons in the atom. The electron becomes a free electron with kinetic energy equal to the difference of the energy lost by the gamma ray and the electron binding energy. Because the binding energy of the electron is negligibly small in comparison to the incident gamma ray energy, the kinetic energy of that electron will be nearly equal to the energy lost by the gamma ray:

$$E_{e^-} = E_\gamma - E' \tag{2.7}$$

where E_{e^-} is the energy of the recoiled electron, E_γ is the energy of the incident gamma ray, E' is the energy of the scattered gamma ray. Only partial energy transfer is allowed for this interaction because of conservation of energy and momentum. Hence, unlike the photoelectric effect, the gamma ray in this interaction is scattered and never fully absorbed.

The interaction of two particles in Compton effect (the photon and the electron) is often compared to billiard balls collisions, where both the striking and target balls deflect at an angle right after collision. The direction of the electron and the gamma ray leaving the interaction site depends on the energy transferred by the incident gamma ray to the electron, as governed by the following equation.

$$E' = \frac{m_0 c^2}{\left(1 - cos\phi + \frac{m_0 c^2}{E_\gamma}\right)} \tag{2.8}$$

where $m_0 c^2$ is the rest energy of the electron (0.511 MeV), ϕ is the angle between the incident and scattered gamma rays, E_γ and E' are the energy of the incident and scattered gamma rays, respectively. The probability of Compton effect occurring is called the *Compton cross section*. It is a complicated function of photon energy, but it may be written in the form:

$$\sigma = NZf\left(E_\gamma\right) \tag{2.9}$$

where σ is the Compton cross section (m^{-1}), $f\left(E_\gamma\right)$ is a function of gamma ray energy, N and Z are density and atomic number of the material respectively [14].

2.1.3. Pair production

In pair production, a gamma ray interacts with the electric field of the nucleus and is converted to an electron-positron pair. This interaction only happens for gamma rays of energies above 1.022 MeV because of energy conservation, as each of the electron and positron have a mass of 0.511 MeV, the energy needed to create this pair must be at least twice as much. The surplus energy of the gamma ray is shared between the electron and positron as kinetic energy. An illustration of pair production is shown in Figure 2.4.

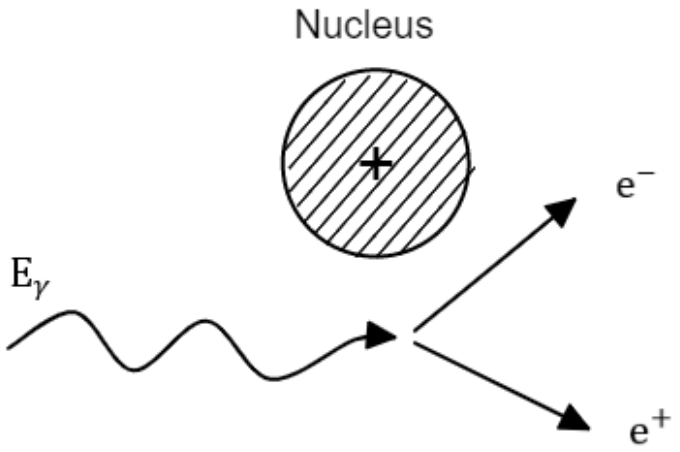

Figure 2.4. Schematic representation of pair production under the influence of a nucleus.

The positron e^+, which is the antiparticle of electron, is rapidly slowed down and will eventually combine with an electron in the absorber, where they both annihilate. The annihilation process releases two gamma rays of 0.511 MeV each, travelling in opposite directions, to conserve momentum. The pair production probability, or cross section, varies with the square of the atomic number Z, and it may be written in the form:

$$\kappa = NZ^2 f(E_\gamma, Z) \tag{2.10}$$

where κ is the probability for pair production to occur per unit distance traveled (m^{-1}), and $f(E_\gamma, Z)$ is a function that changes slightly with Z and increases with E_γ [15, 16].

2.2. Gamma Ray Attenuation

A gamma ray may interact in any of the three main ways mentioned earlier when it travels through matter (though for pair production, it must have an energy higher than 1.022 MeV). Figure 2.5 shows the importance of the three interactions (photoelectric, Compton, and pair production) as the energy of the gamma ray and Z of the target material change.

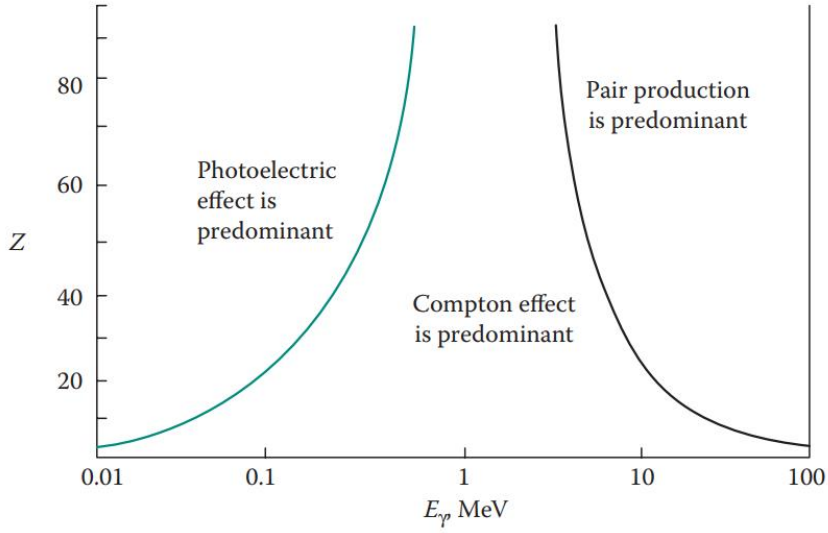

Figure 2.5. The relative importance of the three major gamma ray interactions (from Tsoulfanidis et al. [14]).

It is observed that the interaction of the photoelectric effect is predominant for gamma rays of low energy. For intermediate energies, the interaction of the Compton effect predominates, and for high energies pair production is the dominant interaction. Similarly, the atomic number Z of the absorber material can also decide which interaction is going to be dominant at given energies. Taking a photon of 10 MeV for example, if it is travelling through carbon (Z = 6) the main mechanism of interaction will be the Compton effect. Whereas if the same photon was travelling through iodine (Z = 53) it will interact mostly through pair production.

The total probability of interaction, also known as the *linear attenuation coefficient* μ, is equal to the sum of the probabilities, or cross sections, for each interaction.

$$\mu = \tau + \sigma + \kappa \tag{2.11}$$

where τ, σ and κ are the cross sections for the photoelectric effect, the Compton effect, and pair production respectively. The linear attenuation coefficient is attenuation per unit of distance (cm^{-1}). The use of the linear attenuation coefficient is constrained by the fact that it varies with the density of the absorber. A more favorable parameter is the *mass attenuation coefficient* (μ_m), which normalizes the linear attenuation coefficient by the density of the absorber material. It relates to the linear attenuation coefficient by the following equation.

$$\mu_m = \frac{\mu}{\rho} \tag{2.12}$$

where ρ is the density of the material in $\mathrm{g/cm^3}$. Thus, the mass attenuation coefficient (μ_m) is attenuation per unit mass ($\mathrm{cm^2/g}$).

The intensity of gamma rays decreases exponentially while passing through a medium (Figure 2.6.) according to the Lambert-Beer law.

$$I(t) = I(0)e^{-\mu t} \tag{2.13}$$

where $I(0)$ is the initial intensity of the incident gamma rays, t is the thickness of the medium, and $I(t)$ is the intensity of the emerging gamma rays after travelling a distance t in the medium. The exponential $e^{-\mu t}$ is the probability that a gamma ray will travel through a medium of thickness t without interaction.

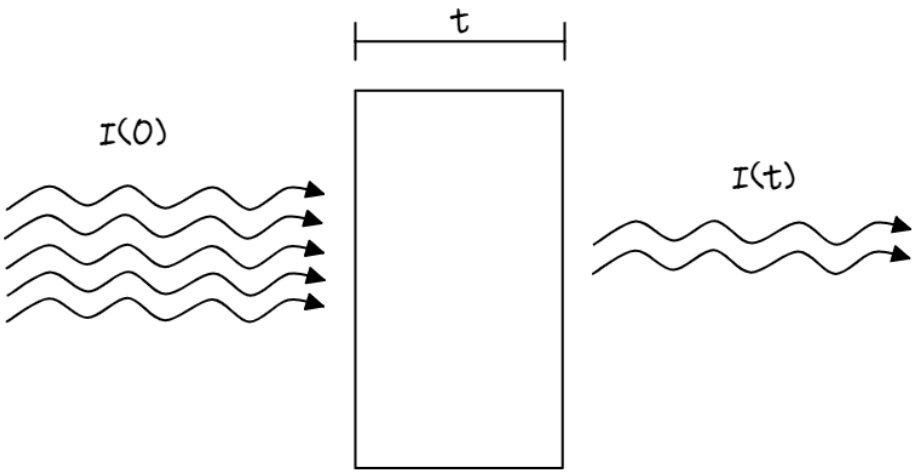

Figure 2.6. The intensity of the transmitted beam decreases exponentially with the material thickness.

The thickness of a given material at which 50% of the incident beam has been attenuated is known as the *half value layer* (*HVL)*. This quantity can be derived from the Lambert-Beer law, and it is important for describing the penetrating ability of gamma rays through materials. The HVL is expressed in units of distance (cm), and it is dependent on the energy of the gamma ray. Solving equation 2.13 for t and setting the fraction $I(t)/I(0)$ to $\frac{1}{2}$, it changes to:

$$HVL\ (cm) = t_{1/2} = \frac{\ln 2}{\mu} \tag{2.14}$$

A similar parameter that is also used in gamma penetration calculations is the *tenth value layer (TVL)*, which is defined as the thickness of a given material of at which the intensity of radiation entering it is reduced to one tenth of its original intensity.

$$TVL\ (cm) = t_{1/10} = \frac{\ln 10}{\mu} \tag{2.15}$$

The HVL and TVL fundamentally share the same concept and their value increases as the energy of the gamma ray increases (inversely proportional to the linear attenuation coefficient). The *mean free path* (λ) also exhibits the same behavior. The mean free path is the average distance a gamma ray travels in a material before an interaction takes place. It is simply the reciprocal of the linear attenuation coefficient.

$$\lambda\ (cm) = \frac{1}{\mu} \tag{2.16}$$

The Lambert-Beer law (equation 2.13) does not account for beam divergence and the multiple scattering of gamma rays (which are due to the large thickness of the interacting medium). For the law to be valid, certain conditions need to be met:

i. The gamma rays need to be monoenergetic.
ii. The interacting medium must be thin.
iii. The gamma rays need to be collimated into a narrow beam (*narrow beam geometry*).

In place of meeting these difficult conditions, a simple multiplicative correction has been introduced, and the law is modified to:

$$I(t) = BI(0)e^{-\mu t} \tag{2.17}$$

where *B* is the correction factor and it's known as the *build-up factor*. B is always greater than or equal to unity, depending on the type of gamma ray detector used and the specific geometry of the experiment (B =1 when the three conditions above are met).

2.3. Gamma Ray Shielding

Shielding simply means having some material between the source of radiation and the person (or some device) that will absorb the radiation. It is one of the practices used to limit exposure to ionizing radiation and reduce possible risks. Materials used for shielding against gamma rays must be of high density and high atomic number because in that way they will have a high linear attenuation coefficient and a high photoelectric absorption probability. Low-density materials and low-Z materials can be compensated for with increased thickness. In the case of shielding materials that consists of various elements, in place of Z, the *effective atomic number* Z_{eff} impacts

the likelihood of photon absorption. The effective atomic number is equivalent to the atomic number Z of an element, but for composite materials. Unlike Z however, which is constant, Z_{eff} is energy dependent (more in section 3.1.2.). Effective atomic number, mass attenuation coefficient, linear attenuation coefficient, HVL, MFP, and build-up factor are all shielding parameters related to gamma rays, often referred to as *GSP* (Gamma Shielding Parameters). The shielding effectiveness of materials can be examined on the basis of these parameters.

Lead (Pb) is commonly used for gamma ray protection for its high density and atomic number. Beside lead, many other materials have been tested for gamma shielding, like concrete [17], alloys [18], and polymers [19]. Glasses are also used, and preferred for their optical transparency, low cost, and ease of formatting [20, 21].

3. METHOD

The working steps of GRASP can be divided into the following categories:

a. Input: Requiring from the user information regarding the composition and density of the material to be studied, in addition to the energy range of interest.
b. Calculation: Extracting the photon cross-section values of the elements which constitute the material from the database. Then, calculating the gamma shielding parameters for the material using built-in equations.
c. Output: Producing tables and graphs which display the results of gamma shielding parameters as functions of energy.

The photon cross sections mentioned in the calculation category are taken from XCOM [4], more on this in section 3.1. The input and output categories are explained in detail in section 3.2, while section 3.3 covers the limitations of the program.

3.1. The Calculation of Gamma Shielding Parameters

For any given material, GRASP can calculate the following gamma shielding parameters: mass attenuation coefficient (MAC), linear attenuation coefficient (LAC), half value layer (HVL), tenth value layer (TVL), mean free path (MFP), and effective atomic number (Z_{eff}). All of the above are energy dependent quantities that need the photon cross-section data of the elements which make up the material, in order to be calculated. One may consider stainless steel, for example. This is an alloy of iron that contains a considerable amount of chromium and sometimes other elements like carbon. To calculate one of the aforementioned GSPs for the alloy, the photon cross sections of each of iron, chromium, and carbon are needed to be known first.

Photon cross sections are freely available on XCOM, an online program which generates cross sections for elements, as well as compounds and mixtures. A user can feed XCOM the complete composition of stainless steel or insert one element at a time. This will redirect them to a generated webpage containing a graphical representation and a grid table of partial and total cross sections for the alloy or the element. For

reference, Figure 3.1 shows the XCOM grid table that would be generated for iron (Z = 26).

Atomic Number : 26

To download data in spreadsheet (array) form, choose a delimiter and use the checkboxes in the table heading. After do

Delimiter:

- (●) space
- ( ) | (vertical bar)
- ( ) tab
- ( ) newline

Download data | Reset

Edge	(required) Photon Energy	Scattering		Photoelectric Absorption	Pair Production		Total Attenuation	
		☐ Coherent	☐ Incoherent	☐	☐ In Nuclear Field	☐ In Electron Field	☑ With Coherent Scattering	☐ Without Coherent Scattering
	MeV	cm^2/g	cm^2/g	cm^2/g	cm^2/g	cm^2/g	cm^2/g	cm^2/g
	1.000E-03	4.537E+00	8.777E-03	9.081E+03	0.000E+00	0.000E+00	9.085E+03	9.081E+03
	1.500E-03	4.241E+00	1.530E-02	3.396E+03	0.000E+00	0.000E+00	3.400E+03	3.396E+03
	2.000E-03	3.933E+00	2.124E-02	1.623E+03	0.000E+00	0.000E+00	1.627E+03	1.623E+03
	3.000E-03	3.354E+00	3.206E-02	5.543E+02	0.000E+00	0.000E+00	5.576E+02	5.543E+02
	4.000E-03	2.849E+00	4.212E-02	2.538E+02	0.000E+00	0.000E+00	2.567E+02	2.539E+02
	5.000E-03	2.421E+00	5.133E-02	1.374E+02	0.000E+00	0.000E+00	1.399E+02	1.374E+02
	6.000E-03	2.065E+00	5.966E-02	8.272E+01	0.000E+00	0.000E+00	8.484E+01	8.278E+01
	7.112E-03	1.745E+00	6.800E-02	5.138E+01	0.000E+00	0.000E+00	5.320E+01	5.145E+01
26 K	7.112E-03	1.745E+00	6.800E-02	4.059E+02	0.000E+00	0.000E+00	4.077E+02	4.060E+02
	8.000E-03	1.542E+00	7.395E-02	3.040E+02	0.000E+00	0.000E+00	3.056E+02	3.041E+02
	1.000E-02	1.201E+00	8.541E-02	1.694E+02	0.000E+00	0.000E+00	1.707E+02	1.695E+02
	1.500E-02	7.458E-01	1.047E-01	5.623E+01	0.000E+00	0.000E+00	5.709E+01	5.634E+01

Figure 3.1. XCOM grid table which shows the partial and total attenuation coefficients for iron.

The "total attenuation" in Fig. 3.1 is the linear sum of all the partial cross sections (scattering, photoelectric absorption, and pair production) as described in the previous chapter with equation 2.11. Since every cross section in the figure have units of cm^2/g, it indicates that they are normalized by the density of the element, and that "total attenuation" in fact means the mass attenuation coefficient (MAC) of that element, not the linear attenuation coefficient (LAC). The partial cross sections can be used to acquire some other shielding parameters, like build-up factor, which depends on the ratio of incoherent scattering over total attenuation. However, the only attenuation relevant to GRASP is the total attenuation (with coherent scattering)[2], which represents MAC of the element. In Figure 3.1, this column is distinguished by a tick mark.

[2] Total attenuation coefficients *without* coherent scattering can be used for gamma ray transport calculations.

The total attenuation coefficient data of every featured element ($Z \leq 100$) are collected from XCOM in advance for the preparation of GRASP and are stored as a database in a local directory. Meaning, when the MAC of an element is required, GRASP does not visit the XCOM webpage in real time, as they are not linked together. Instead, it consults its own database, where it obtains the energy dependent MAC values of that element independently. This difference leads to the limitation that is covered in section 3.3.1. Continuing with the stainless-steel example, once GRASP identifies the constituting elements (iron, chromium, and carbon), it explores the database and finds the MAC of these elements. It would now be ready to calculate MAC of the alloy.

3.1.1. Calculation of MAC, LAC, HVL, TVL, and MFP

The calculation of MAC for a composite material (a compound or a mixture) is done by using the mixture rule [22]:

$$(\mu_m)_{\text{mixture}} = \sum_i w_i (\mu_m)_i \tag{3.1}$$

where $(\mu_m)_{\text{mixture}}$ is the MAC of the mixture, $(\mu_m)_i$ is the MAC of the i^{th} element in the mixture, available in the database of GRASP, and w_i is the *weight fraction* of that element, which is provided by the user (section 3.2.1.). The weight fraction of an element is defined as the ratio of its mass (m_i) to the total mass of the mixture/compound (m_{total}):

$$w_i = \frac{m_i}{m_{\text{total}}} \tag{3.2}$$

Next, the linear attenuation coefficients can be obtained from equation 2.12, which requires the density of the material. The user provides the density in units of g/cm^3 (section 3.2.1.). Linear attenuation is the basic shielding parameter from which additional parameters, such as mean free path, half and tenth value layers, are derived. MFP is the reciprocal of the linear attenuation coefficient, as seen from equation 2.16, while HVL and TVL are calculated from equations 2.14 and 2.15, respectively. Details on these parameters are given in section 2.2.

3.1.2. Calculation of Z_{eff}

The effective atomic number of a material made up of different elements cannot be expressed by a single number [23], because unlike Z of an element, Z_{eff} of a composite target material depends on energy of the gamma ray striking it. The method used to

calculate Z_{eff} in this work involves calculation based on the energy dependent MAC values of elements, the equation is adopted from Manohara [24]:

$$Z_{\text{eff}} = \frac{\sum_i f_i A_i (\mu_m)_i}{\sum_j f_j \frac{A_j}{Z_j} (\mu_m)_j} \tag{3.3}$$

where A_i is the atomic weight [25], Z_i is the atomic number, $(\mu_m)_i$ is the mass attenuation coefficient of the i^{th} element in the mixture, and f_i is the *molar fraction* of the i^{th} element, defined as:

$$f_i = \frac{n_i}{n} \tag{3.4}$$

where n_i is the number of atoms of i^{th} element in a compound/mixture, and n is the total number of atoms in that compound/mixture.

$$n = \sum_j n_j \tag{3.5}$$

The molar fraction of an element can be deduced from the chemical formula if the material is a single compound, by using equation 3.4. For example, a water molecule consists of one oxygen atom, and two hydrogen atoms. Their sum is three, thus: $f_{\text{O}} = \frac{1}{3}$ and $f_{\text{H}} = \frac{2}{3}$. If the material is a mixture, the molar fraction can be calculated similarly by applying equations 3.4 and 3.5. For example, water and salt, with the arbitrary percentages of 96% and 4% [$96H_2O + 4NaCl$], the molar fractions would be:

$$n = \sum_j n_j \ = n_{\text{H}} + n_{\text{O}} + n_{\text{Na}} + n_{\text{Cl}} \,,$$

$$n = 192 + 96 + 4 + 4 = 296 \,.$$

therefore,

$$f_{\text{H}} = \frac{192}{296} \approx 0.648 \,,$$

$$f_{\text{O}} = \frac{96}{296} \approx 0.324 \,,$$

$$f_{\text{Na}} = f_{\text{Cl}} = \frac{4}{296} \approx 0.014 \,,$$

and,

$$\sum_i f_i = f_{\text{H}} + f_{\text{O}} + f_{\text{Na}} + f_{\text{Cl}} = 0.648 + 0.324 + 0.014 + 0.014 = 1 \,.$$

Finally, if the material inserted by the user is composed of only one element, then equation 3.3 naturally reduces to Z of that element, a constant.

3.2. GRASP

The GRASP program is available upon request. It is only compatible with Windows for the time being. It runs entirely on the console, without a graphical user interface. The working environment of GRASP is within one directory, containing many files and subfolders that do not require interaction from the user, except for a few: the "*GRASP.exe*" file which executes the program, the "*input.txt*" file which controls the input, and a "*ReadMe.txt*" file which gives instructions to the user and can be used as help. Figure 3.2 displays the content found in the "ReadMe.txt" file. Additionally, there is the empty folder "*saved_data*", which serves as the destination directory for the output tables saved by the user.

```
On the "input.txt" file, you can specify the material according to the following:
Line 1: name of the material
Line 2: fraction by mole or weight: [m/w]
Line 3: the material composition in terms of element symbols (E*) and fractions (F**): [ F1E1 + F2E2 + ... + FnEn ]
Line 4: density of the material in g/cm^3 (***)
Line 5: the energy range in MeV, must be from the list of common energies (****). Maximum range: 0.001-100000
Line 6: option to view plots: [yes/no] or [y/n]

Example:
water
w
11.1898H + 88.8102O
1
0.01-1000
yes

After saving the changes (Ctrl + s), you can run the program by double clicking on "GRASP.exe".
When the program finishes, you can save the data as an Excel file. Saved Excel files are found in the folder "saved_data".
-----------------------------------------------------------------
*     Symbols are case sensitive. Only elements 1-100 are available.
**    If the fractions don't add up to 1, they will be renormalized.
***   Density is required to calculate LAC and its derivatives. MAC and Zeff are independent of density, but Line 4 should NOT be left blank.
****  List of common energies (MeV):
[0.001, 0.0015, 0.002, 0.003, 0.004, 0.005, 0.006, 0.008, 0.01, 0.015, 0.02, 0.03, 0.04, 0.05, 0.06, 0.08, 0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6,
0.8, 1, 1.022, 1.25, 1.5, 2, 2.044, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 20, 22, 24, 26, 28, 30, 40, 50, 60, 80, 100, 150, 200,
300, 400, 500, 600, 800, 1000, 1500, 2000, 3000, 4000, 5000, 6000, 8000, 10000, 15000, 20000, 30000, 40000, 50000, 60000, 80000, 100000]
```

Figure 3.2. The "ReadMe.txt" file.

3.2.1. Input

The input provides the necessary information to the program, like the composition of the material, the density, and the energy range. GRASP reads input from a separate text file which the user can modify according to the instructions. The text file is named "input.txt". A sample input is shown in Fig. 3.3.

```
Water
w
11.1898H + 88.8102O
1
0.01-1000
n
```

Figure 3.3. Default input sample on "`input.txt`". The material is water, expressed in weight fractions (from ICRU Report 44 [26]).

To understand the formatting of the input, the user can refer to the instructions in "`ReadMe.txt`", which clarify that "`input.txt`" should contain six lines as follows:

i. Line 1 is reserved for the name of the material. The name is not relevant to the calculation, but it can serve as an identifier for the material when the data is saved.

ii. Line 2 determines how the material is expressed in terms of fraction, it could be molar fraction or weight fraction. The user types either "`w`" for weight or "`m`" for molar.

iii. Line 3 is for material composition. It is written in terms of elements and fractions, according to the following expression:

$$F_1E_1 + F_2E_2 + \cdots + F_nE_n$$

where F_n and E_n are the fraction and symbol of the n^{th} element, respectively. If the fractions do not add up to 100 or unity, GRASP renormalizes them so that $\sum F = 1$. As an example, *polyboron* [27], which consists of hydrogen, oxygen, carbon, and boron, can be written in the input with the following expression (fraction by weight):

```
12.38H + 22.85O + 59.88C + 4.89B
```

The fraction sum of the above example is 100 as expected. At this stage, GRASP can recognize the elements and access their MACs through its database. The weight fractions are used in equation 3.1 to calculate the MAC of the material. For calculations of Z_{eff}, the molar fractions of the elements are required as demonstrated in equation 3.3. If the user has expressed the material

with weight fractions, the program can convert them to molar fractions as needed, and vice versa, using the following conversion:

$$w_i = f_i \cdot A_i \tag{3.6}$$

where w_i, f_i and A_i are weight fraction, molar fraction, and mass number of the i^{th} element, respectively. The mass numbers of elements are taken from NIST's periodic table of elements [25].

An additional, alternative expression of the material in terms of compounds, is also recognized by GRASP. It is written as follows:

$$f_1 C_1 + f_2 C_2 + \cdots + f_n C_n$$

where C_n is the n^{th} compound of the material, and f_n is the molar fraction of that compound. Numbers are written in-line, the "+" sign separates each compound from the other, while extra spaces are eliminated automatically. This expression only works if the fractions are by mol; Line 2 must read "m". For example, the glass system containing bismuth trioxide, boron trioxide, sodium oxide, magnesium oxide, and barium oxide as fabricated by Sayyed et al. [28] can be expressed as follows (fraction by mol):

```
0.3Bi2O3 + 0.2BaO + 0.1Na2O + 0.1MgO + 0.3B2O3
```

iv. Line 4 determines the density of the material in units of $\mathrm{g/cm^3}$. The density is required for the calculation of LAC, and the other parameters which are derived from it (HVL, TVL, and MFP). If the user is only interested in Z_{eff} for example, which is independent of density, they can type-in any number in this line as a placeholder (leaving Line 4 blank will give an error). The user should be warned that the LAC of the material will no longer be accurate when this is done.

v. Line 5 determines the energy range, with an expression of two numbers (in units of MeV) and a hyphen in-between, written like "`0.02-1.5`". This range expression contains the energies from 0.02 MeV to 1.5 MeV (both ends included). The maximum range is "`0.001-100000`", analogous to XCOM.

vi. Line 6 regards the plots, whether the user wishes to view them or not. It is a yes or no input ("`y`" = yes, "`n`" = no).

GRASP can only work with one material at a time. If the user attempts to calculate the shielding parameters for a second material, they need to replace the information on the input file with that of the second material, and so on. When the complete information of a material is inserted on "`input.txt`", the user can save the changes and run the program by executing "`GRASP.exe`".

3.2.2. Output

GRASP provides tables and graphs for its output; the tables appear in the console, while the graphs appear in windows of their own.

3.2.2.1. Tabular Output

Two tables are displayed, the first contains the composition of the material in terms of the elements and their respective atomic numbers, mass numbers, and (normalized) fractions by mol and weight. On top of this table the name of the material and its density appear. The second table contains the calculated values of the gamma shielding parameters as functions of gamma ray energy. Figure 3.4 shows the tabular output for bone-equivalent plastic (B-100) in the range 0.001 – 0.015 MeV, as would appear in the terminal.

```
Sample name: 'Bone-equivalent plastic (B-100)',         density = (1.45 g/cm³),         composition:

 element   |   Z |      A |   fraction by mol |   fraction by weight
-----------+-----+--------+-------------------+----------------------
 H         |   1 |  1.008 |           0.5138  |              0.06547
 C         |   6 | 12.011 |           0.3536  |              0.5369
 N         |   7 | 14.007 |           0.01214 |              0.0215
 O         |   8 | 15.999 |           0.01586 |              0.03208
 F         |   9 | 18.998 |           0.06971 |              0.1674
 Ca        |  20 | 40.078 |           0.03485 |              0.1766

Gamma shielding parameters:

+------+-------------+-------------+-----------+-----------+-----------+-----------+-----------+
| Edge | Energy (MeV) | MAC (cm²/g) |   Zeff    | LAC (1/cm) | HVL (cm)  | TVL (cm)  | MFP (cm)  |
+------+-------------+-------------+-----------+-----------+-----------+-----------+-----------+
|      |  1.000e-03  |  3.211e+03  | 8.564e+00 | 4.656e+03 | 1.489e-04 | 4.945e-04 | 2.148e-04 |
|      |  1.500e-03  |  1.083e+03  | 8.713e+00 | 1.570e+03 | 4.414e-04 | 1.466e-03 | 6.368e-04 |
|      |  2.000e-03  |  4.878e+02  | 8.822e+00 | 7.073e+02 | 9.800e-04 | 3.255e-03 | 1.414e-03 |
|      |  3.000e-03  |  1.542e+02  | 8.982e+00 | 2.236e+02 | 3.099e-03 | 1.030e-02 | 4.472e-03 |
|      |  4.000e-03  |  6.717e+01  | 9.094e+00 | 9.739e+01 | 7.117e-03 | 2.364e-02 | 1.027e-02 |
|      |  4.038e-03  |  6.534e+01  | 1.484e+01 | 9.475e+01 | 7.316e-03 | 2.430e-02 | 1.055e-02 |
| 20 K |  4.038e-03  |  2.250e+02  | 1.484e+01 | 3.263e+02 | 2.124e-03 | 7.057e-03 | 3.065e-03 |
|      |  5.000e-03  |  1.298e+02  | 1.517e+01 | 1.882e+02 | 3.683e-03 | 1.223e-02 | 5.313e-03 |
|      |  6.000e-03  |  7.941e+01  | 1.535e+01 | 1.151e+02 | 6.020e-03 | 2.000e-02 | 8.684e-03 |
|      |  8.000e-03  |  3.620e+01  | 1.555e+01 | 5.248e+01 | 1.321e-02 | 4.387e-02 | 1.905e-02 |
|      |  1.000e-02  |  1.944e+01  | 1.554e+01 | 2.819e+01 | 2.459e-02 | 8.168e-02 | 3.547e-02 |
|      |  1.500e-02  |  6.221e+00  | 1.490e+01 | 9.021e+00 | 7.684e-02 | 2.552e-01 | 1.109e-01 |
+------+-------------+-------------+-----------+-----------+-----------+-----------+-----------+
```

Figure 3.4. Tabular output for bone-equivalent plastic (B-100) by GRASP.

It is seen that in the leftmost of the second table there is a column labeled "`Edge`", just before the energy column. The purpose of this column is to identify absorption edges (see section 3.3.2.) existing in the range if any, by stating the atomic numbers of the responsible elements, and the name of the electron shells (K, L, or M). For the material featured in Figure 3.4., there is one K-edge in the range, located at 0.004038 MeV. It is due to calcium (Z = 20).

3.2.2.2. Graphical output

Graphical representations of the shielding parameters are optional, they can be enabled or disabled from Line 6 in the "`input.txt`" file (section 3.2.1.). Figures 3.5, 3.6, and 3.7 show the windows containing graphs of different shielding parameters for water, as produced by GRASP.

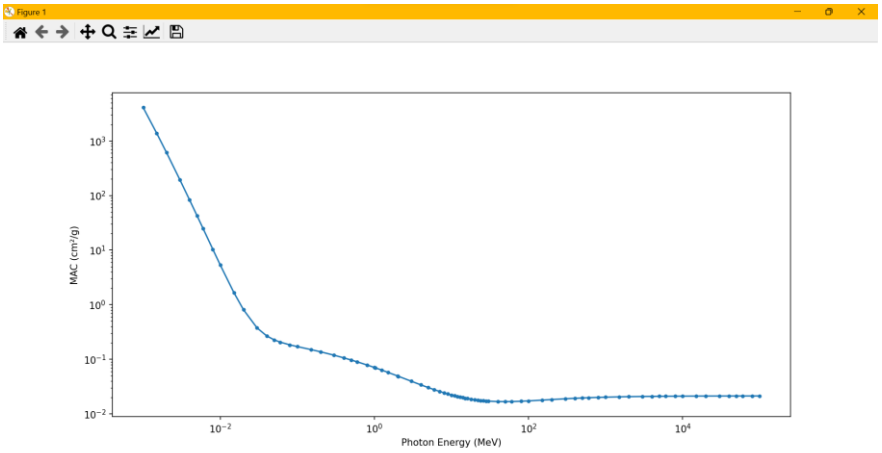

Figure 3.5. Graphical representation of MAC for water as calculated by GRASP.

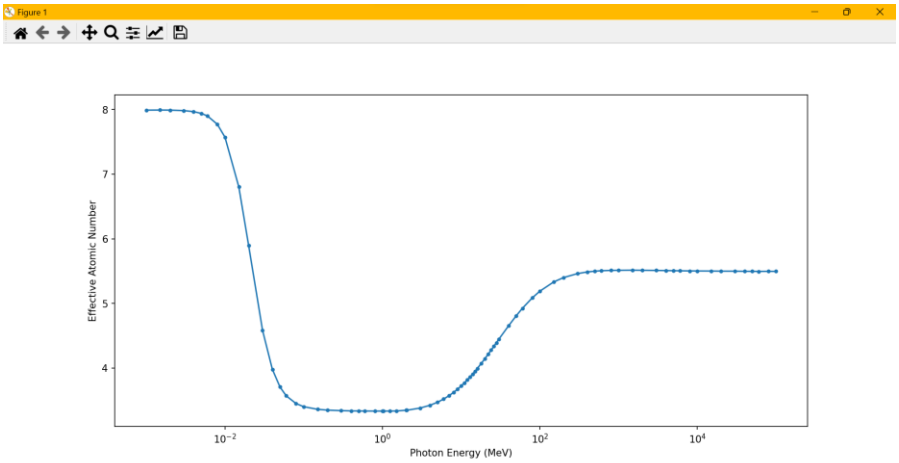

Figure 3.6. Graphical representation of Z_{eff} of water as calculated by GRASP.

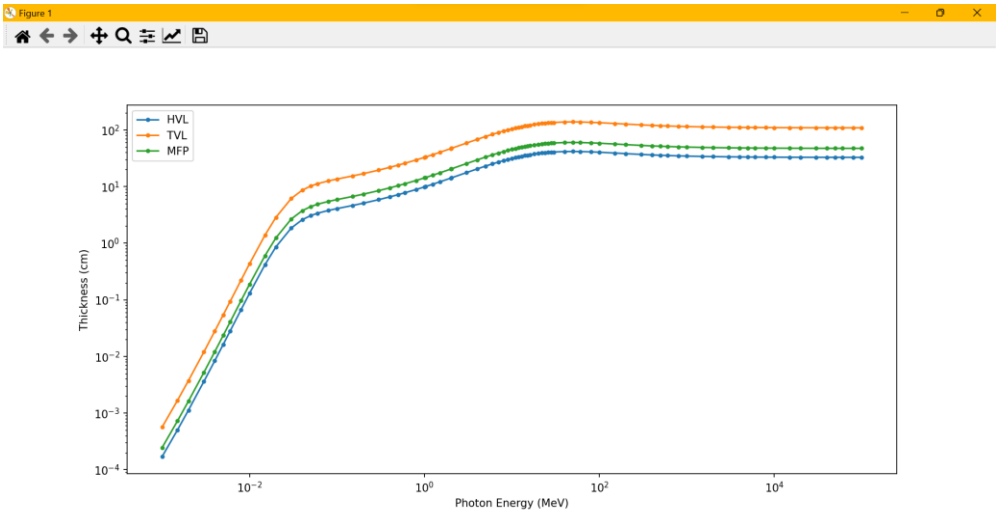

Figure 3.7. Graphical representation of HVL, TVL, and MFP of water as calculated by GRASP.

3.2.3. Saving data

3.2.3.1. Saving the tables

After displaying the output, GRASP prompts the user a question in the terminal:

"`Save data? (y/n) --->` "

to which can be replied with either "y" (for yes) or "n" (for no). If the answer is affirmative, an Excel file is created inside the folder "saved_data", which is located in the main directory of GRASP. The created file is identified by the name of the material followed by the extension ".xlsx". The name is set previously by the user in Line 1 on "input.txt" (section 3.2.1.). For example, if the user sets the name of the material to "sample_1", the created file will be named "sample_1.xlsx". If there already exists a file with this name inside the "saved_data" folder, GRASP will not overwrite the data. Instead, it will abort the saving command and show the following message:

```
Error: "sample_1.xlsx" file already exists. Consider
changing the name of the material (Ln 1 on "input.txt")
```

Figure 3.8. shows the contents of a newly produced Excel file by GRASP for a sample material. The data of each shielding parameter is presented on a different sheet, and there is a sheet dedicated to the composition of the material. Thus, a total of seven sheets are found in the Excel file: "Composition", "MAC", "LAC", "Zeff", "HVL", "TVL", and "MFP".

	A	B	C	D
1	Energy (MeV)	Zeff		
2	0.001	8.563728763		
3	0.0015	8.712899842		
4	0.002	8.821910106		
5	0.003	8.981219513		
6	0.004	9.093933866		
7	0.004038	14.82756537		
8	0.004038	14.82756537		
9	0.005	15.16589334		
10	0.006	15.35277115		
11	0.008	15.54928559		
12	0.01	15.5434708		
13	0.015	14.90265297		
14	0.02	13.61666446		

Composition | MAC | LAC | Zeff | HVL | TVL | MFP

Figure 3.8. Excel sheet produced by GRASP for a sample material.

3.2.3.2. Saving the graphs

The graph outputs are displayed in interactive windows that contain a number of buttons, one of which is a saving button (Figure 3.5). While on display, the user can also navigate regions of the plot by using the zooming tool. Once saved, however, the plots change into fixed images and lose their interactive tools. A GRASP graph can be saved in a variety of dynamic graphic formats such as PNG, JPG, EPS, PDF, etc. The user decides the name and destination of the saved graph file.

3.3. Limitations

3.3.1. Standard energy grid

GRASP follows the semi-logarithmic spacing of energies presented in a default XCOM energy-grid, meaning, the range of energies misses some points that would have existed on a linear scale. For example, when the user narrows the energy range to "0.1–1" MeV in GRASP, the list of energies will include the following values [0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1.0] and exclude other values like [0.7, 0.9], or [0.25, 0.35, …]. GRASP does not feature these energies because it blindly follows the standard XCOM energy-grid from 1 keV to 100 GeV, which is the maximum range. It contains the following energies common to all the elements, and are referred to as the *standard energies* (in MeV) throughout this thesis:

[0.001, 0.0015, 0.002, 0.003, 0.004, 0.005, 0.006, 0.008, 0.01, 0.015, 0.02, 0.03, 0.04, 0.05, 0.06, 0.08, 0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1, 1.022, 1.25, 1.5, 2, 2.044, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 20, 22, 24, 26, 28, 30, 40, 50, 60, 80, 100, 150, 200, 300, 400, 500, 600, 800, 1000, 1500, 2000, 3000, 4000, 5000, 6000, 8000, 10000, 15000, 20000, 30000, 40000, 50000, 60000, 80000, 100000]

Therefore, when the user sets a range, they must start and end with a standard energy, otherwise the program will give an error.

This is a dependency problem. If GRASP could compute attenuation data of elements on its own, it would be able to manage any energy within XCOM's range. One of the

benefits of that is being able to calculate attenuation at decay energies of gamma ray sources. For example, Cs-137 is a radioactive isotope which emits 0.6617 MeV gamma rays (Figure 2.1.), GRASP does not feature this energy. The closest standard energy to it is 0.6 MeV. It is worth noting that in XCOM, one could manually insert any energy (must have a maximum of four significant figures) and get attenuation results for it if it is within the range of 1 keV to 100 GeV.

3.3.2. Absorption edges

The *absorption edge* is a sudden increase in the attenuation which is caused by photoelectric absorption. It occurs when the photon has an energy that is slightly above the binding energy of an electron. A photon with that energy is more likely to be absorbed than one that has an energy slightly below the binding energy or far above it [29]. The terms *K-edge*, or *L-edge* refer to the absorption edges of the K-shell and the L-shell of an atom, and so on. For example, the K-edge of lead is at 0.088 MeV. Lighter elements, like carbon, do not have an absorption edge in the range 1 keV – 100 GeV. Any element that has an absorption edge in its default XCOM energy grid, will also have those energies in GRASP. This makes the attenuation data uneven from element to element, as some of them do not have energies corresponding to absorption edges.

In the case of a material composed of lead and other elements, equation 3.1 would not be solved at 0.088 MeV (K-edge of lead), unless the attenuation data for those other elements are provided at that energy as well. In the default XCOM grid, the energy 0.088 MeV does not exist for elements other than lead. In other words, GRASP has to produce attenuation values for the other elements at this particular energy, and at other absorption energies when needed. This is explained more clearly in the following example.

Consider a tungsten-copper alloy ("`0.65W + 0.35Cu`" by weight). The K-edge of copper is at 0.008979 MeV. This energy is unique to copper and is not available in GRASP's database of tungsten. Therefore, when calculation is made based on the data obtained from XCOM, no mass attenuation coefficients are determined at the absorption edges of copper. One of the ways to overcome this deficiency is to estimate the attenuation values at the absorption edge by averaging the values belonging to the energies adjacent to the absorption edge of interest. In this example, the absorption edge is the K-edge of copper (0.008979 MeV) lies between 0.008 and 0.01 MeV, two

energies with available attenuation values in the database of tungsten, the ‘midpoint’ is 0.009 MeV, which is close to the K-edge of interest, as shown in Figure 3.9.

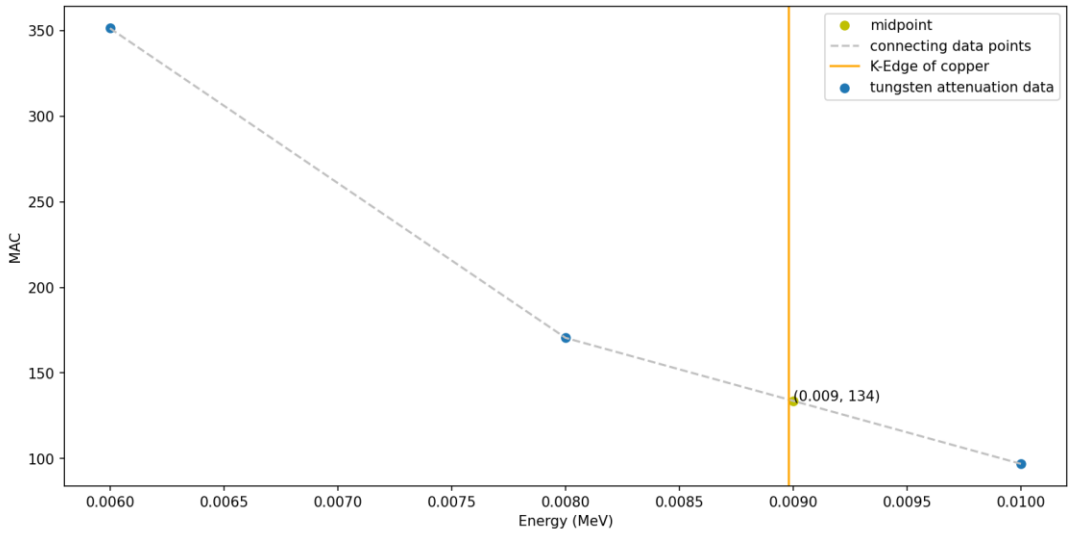

Figure 3.9. “Midpoint” solution to the unavailability of attenuation data of tungsten at the energy corresponding to the K-edge of copper.

Thus, a reasonable answer 134 $\frac{cm^2}{g}$ is obtained. However, absorption edges are not always near the midpoints. Tungsten, for example, has the edges 0.01021, 0.01154, and 0.01210 MeV, which belong to L3, L2, and L1, respectively (Figure 3.10.).

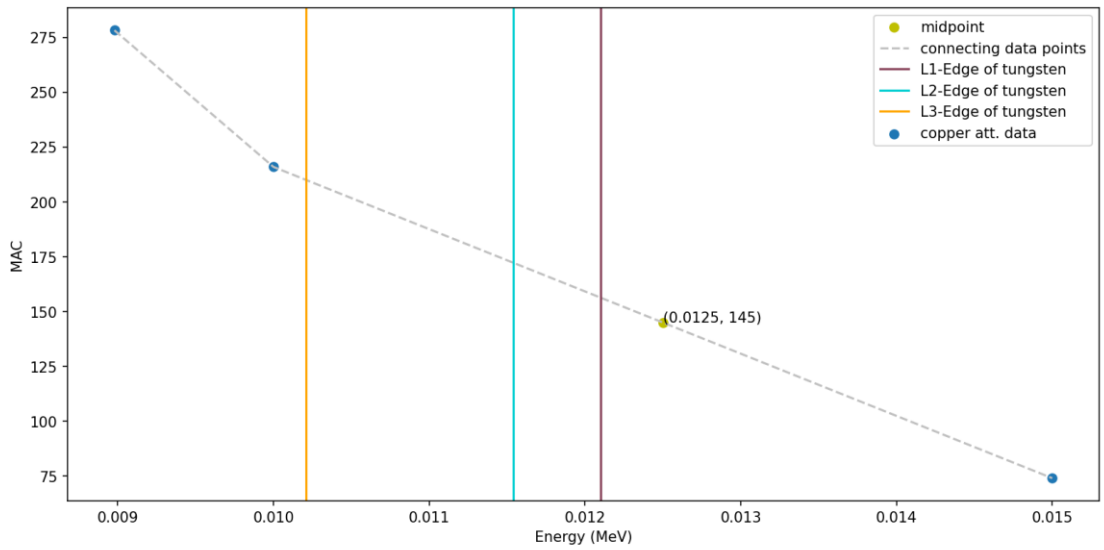

Figure 3.10. The energies corresponding to the L-edges of tungsten are not close to the midpoint created by GRASP.

Since all these edges are positioned between 0.01 and 0.015 MeV, they would have the same midpoint at 0.0125 MeV, and in return each gives the same average attenuation value (145 $\frac{cm^2}{g}$). Hence, the midpoint solution does not provide results with satisfactory precision. A better solution to the absorption-edge problem is making an exponential fit to the data at the absorption edge region. Such fit using GRASP is shown in Figure 3.11.

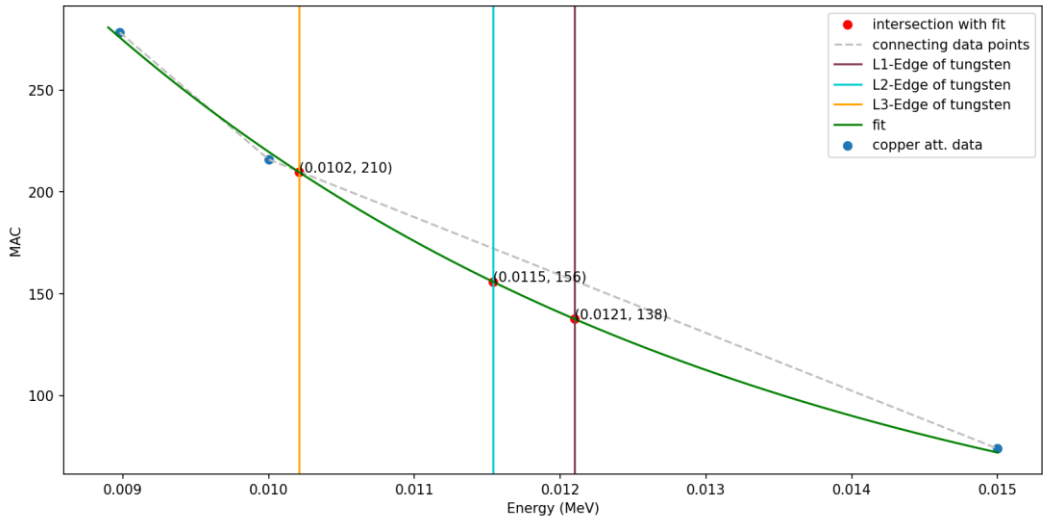

Figure 3.11. The decay-exponential fit GRASP employs to find the attention values of copper at the energies corresponding to L-edges of tungsten.

It is observed in Figure 3.11 that the exponential fit gives each L-edge a unique and reasonable attenuation value: 209.7, 155.9, and 137.6 cm^2/g for L3, L2, and L1, respectively. In comparison with XCOM (205.3, 150.4, and 132.7 $\frac{cm^2}{g}$ for L3, L2, and L1), the average deviation is 3.16% in this example. Depending on the element in the material and energy of the absorption edge, the discrepancy between XCOM and GRASP's exponential fit, in general, may vary from about less than 0.2% a minimum, up to about 8.5% a maximum.

For a certain absorption edge energy with missing attenuation value, GRASP performs this fitting by involving the three nearest to the edge energies with available values. In the latest example of the L-edges, the three nearest energies are: 0.008979, 0.01, and 0.015 MeV (represented in Figure 3.11 with blue dots). There are two reasons why involving three energies could practically lead to the best curve:

i. It is found that the wider the range is, the more offside the curve will appear in general. That is, the more energies are involved in the fit, the less accurate the results will be, concerning the expected attenuation values at the absorption edges. So, a fit involving three nearby energies is slightly better than another involving five, and much better than a fit involving ten.

ii. Some absorption energies are located near the very first standard energies, for instance, between 0.001 and 0.0015 MeV. In such situations, GRASP cannot involve energies from both sides evenly: no data is found below 0.001 MeV. In consequence, the resulting curves will be of poor quality if they involve many energies in their range (for example, 0.001 – 0.006 MeV), especially for this sensitive region where the drop in attenuation is within orders of magnitude.

3.3.3. Z_{eff} and absorption edges

For each energy corresponding to an absorption edge, GRASP receives two MAC values, one low value that continues the trend of falling, and one high value which gives the plotline a spike. GRASP only employs the higher MAC value for the Z_{eff} equation (equation 3.3), which is the value responsible for the edge, while the lower MAC value is dropped. This is done so as to consistently get one Z_{eff} value for each energy, avoiding multivalued solutions. While the discontinuity of MAC points to the shell structure of a certain element, there is no equivalent physical meaning for a discontinuity in Z_{eff} which can be consistent with the intent of an effective atomic number concept. This action by GRASP, however, may increase the uncertainties of Z_{eff} near the absorption edges (section 4.2.).

On a related note, the Auto-Zeff software [5] also faces multiple values at absorption edges, but it picks the one value corresponding to the smoothest Z_{eff} curve.

4. RESULTS

In this work a new program, GRASP, has been developed using Python, an object oriented, all-purpose programming language. GRASP can calculate some gamma shielding parameters for any specified material. The working procedure of the program and the role of the user have been described in the previous chapter. Analysis of some shielding parameters for various materials available in the literature have been done using GRASP, and the results are discussed in this chapter. In addition, the results have been compared with those obtained using other programs.

4.1. Mass Attenuation Coefficients

Because GRASP takes energy dependent attenuation values for the elements of interest from XCOM, its calculation of MAC for composite media (equation 3.1) is expected to be in a complete agreement with that of XCOM, with deviations only near energies of absorption edges, due to GRASP's improvised fitting in these regions (section 3.3.2.). For validity, a sample of three glasses of lead-free silica borotellurite containing various amounts of bismuth trioxide [30] is studied. Table 4.1. shows the composition and density of these glasses.

Table 4.1. The composition and density of some lead-free silica borotellurite glasses containing bismuth oxide [30].

Sample	Density	Chemical oxides (% mol)			
	(g/cm^2)	TeO_2	B_2O_3	SiO_2	Bi_2O_3
BSBT3	4.10	54.32	23.28	19.40	3.00
BSBT4	4.15	53.76	23.04	19.20	4.00
BSBT5	4.30	53.20	22.80	19.00	5.00

The mass attenuation coefficients of glasses BSBT3, BSBT4, and BSBT5 are calculated by GRASP and compared to the results by XCOM in Table 4.2, for the

range of 0.01 – 0.15 MeV. The table also contains data from FLUKA, a Monte Carlo simulation package for the interaction of particles and nuclei in matter [31]. FLUKA is widely used as an effective alternative for investigating the physical parameters when the experimental preparations are limited or difficult to reach [32].

Table 4.2. Mass attenuation coefficients as calculated by XCOM, GRASP, and FLUKA.

Energy	Mass Attenuation Coefficient (cm^2/g)								
	BSBT3			BSBT4			BSBT5		
(MeV)	XCOM	GRASP	FLUKA	XCOM	GRASP	FLUKA	XCOM	GRASP	FLUKA
0.01	97.37	97.36	97.08	98.28	98.29	98.14	99.17	99.16	99.31
0.01342	44.50 53.40	47.85 56.74	46.24	45.01 56.55	48.24 58.29	47.10	45.40 59.55	48.61 62.66	48.15
0.015	39.67	39.67	39.73	42.01	42.02	41.87	44.24	44.25	44.21
0.01571	35.03 38.83	35.43 39.23	35.68	37.11 42.04	37.50 42.43	37.90	39.09 45.09	39.46 45.46	40.17
0.01639	34.83 36.73	35.59 37.49	35.34	37.75 40.22	38.48 40.95	38.38	40.52 43.53	41.23 44.24	41.34
0.02	21.80	21.80	21.71	23.93	23.93	23.80	25.95	25.95	25.90
0.03	7.498	7.499	7.442	8.254	8.256	8.173	8.973	8.975	8.888
0.03181	6.429 22.85	6.489 22.91	20.49	7.078 22.91	7.156 22.99	20.60	7.695 22.96	7.789 23.05	20.72
0.04	12.70	12.70	12.69	12.73	12.73	12.72	12.75	12.76	12.73
0.06	4.380	4.380	4.379	4.392	4.392	4.421	4.404	4.404	4.409
0.08	2.063	2.064	2.068	2.071	2.072	2.067	2.079	2.079	2.075
0.09053	1.503 2.042	1.559 2.098	1.714	1.509 2.209	1.563 2.263	1.833	1.516 2.367	1.568 2.420	2.149
0.1	1.588	1.588	1.583	1.718	1.718	1.720	1.841	1.841	1.841
0.15	0.603	0.603	0.600	0.649	0.649	0.652	0.693	0.693	0.692

It is observed that GRASP's results are nearly equal to that of XCOM, except at the absorption edges where they deviate noticeably. This deviation can be explained by the fitting done by GRASP; estimating the attenuation of the elements which do not have it at the absorption edges of others (section 3.3.2). Whereas in standard energies, the results of GRASP should agree with XCOM since it is borrowing data directly from XCOM's standard energy grid of elements. Overall, the deviation averages

1.34%. The discontinuity of MAC as given by XCOM at absorption energies, is also seen in GRASP, whereas FLUKA gives a singular value at these energies. FLUKA performs a simulation of the transmission of gamma rays in these glasses, in a narrow beam geometry environment. It then obtains the linear attenuation values from the Lambert-Beer law (equation 3.13), and by knowing the density of the glasses as provided in Table 4.1, MAC can be found directly from equation 2.12. It can be seen that FLUKA's result is also in good agreement with the theoretical values of XCOM.

Comparisons of other parameters that are directly derived from mass attenuation coefficient, like LAC, MFP, or HVL, mirror what have been stated above. The other gamma shielding parameters, except for Z_{eff}, are obtained using simple conversions, as seen from equations 2.12, 2.14, 2.15, and 2.16. Namely, for example, to evaluate the mean free path MFP of a glass, the MAC results given by XCOM, FLUKA, and GRASP are taken from Table 4.2. and multiplied by the density of that glass to obtain the linear attenuation coefficients LAC (equation 2.12), then the reciprocal of LAC provides the MFP values for the glass of interest (equation 2.16). GRASP does this calculation automatically as explained in section 3.1.1 since it already provides every parameter at once. The findings for BTSB3 glass, for instance, are graphically illustrated in Figure 4.1.

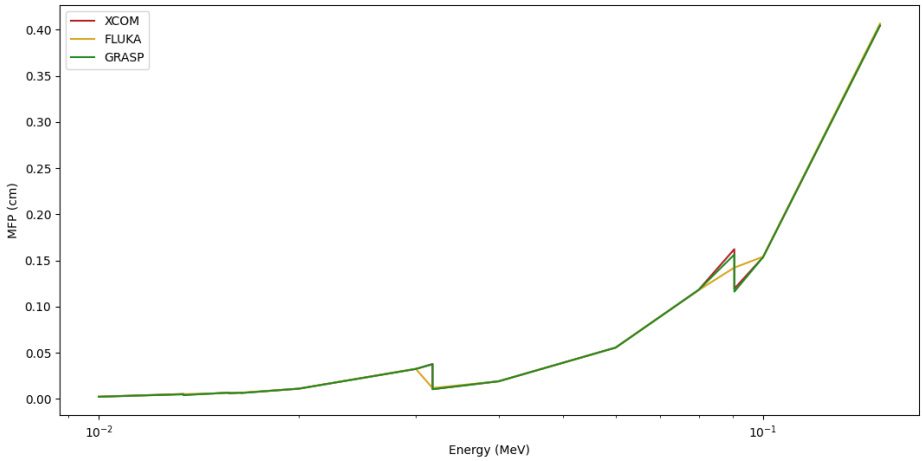

Figure 4.1. The mean free path of BTSB3, as evaluated using MAC values given by XCOM, FLUKA, and GRASP.

The three plotlines overlap across the entire range, except for the energies corresponding to the absorption edges. Even there, GRASP and XCOM values deviate

slightly, whereas the single value given by FLUKA sets it apart. It can be concluded that, regarding MAC and its direct derivatives (LAC, MFP, HVL, TVL), the results of GRASP are in good agreement with those of XCOM. In the standard energies it matches XCOM, and the fitting procedure done to include absorption edges is decently valid.

4.2. Effective Atomic Numbers

In order to validate GRASP's calculation of Z_{eff}, results of the calculations are compared to those of Phy-X/PSD and the Auto-Zeff software. The former calculates Z_{eff} using the direct method, similar to GRASP, characterized by equation 3.3. While the latter calculates Z_{eff} using a more complicated interpolation process which involves different methods for different energy regions [5]. The comparison is carried out in two stages. First, a sample material is chosen which consists of heavy elements, so as to analyze the performance of GRASP regarding absorption edges. Second, a different sample consisting of lighter elements is studied, one which does not exhibit any characteristic absorption edges in the energy range of interest.

The sample selected for stage one is a casting gold alloy commonly used for teeth restoration. Let the name of the alloy be Alloy-A, as taken from Bergman [33]. The formula of Alloy-A as provided by the manufacturer is:

$$74Au + 10.5Ag + 11Cu + 0.5Pt + 3.5Pd + 0.5Zn$$

Table 4.3 presents the Z_{eff} data of Alloy-A as calculated by the three programs in the full range of Auto-Zeff (0.01 – 1000 MeV).

Table 4.3. The effective atomic number for Alloy-A as calculated by Auto-Zeff, GRASP, and Phy-X/PSD.

Energy (MeV)	Effective Atomic Number		
	Auto-Zeff	GRASP	Phy-X
0.01	73.96	55.67	55.67
0.01156	50.74	61.92	-
0.01192	50.51	64.82	-
0.01239	59.76	63.50	-
0.01279	59.61	64.72	-
0.01327	59.77	65.11	-
0.01357	59.92	65.63	-
0.01373	59.99	67.64	-

Table 4.3. (Continued) The effective atomic number for Alloy-A as calculated by Auto-Zeff, GRASP, and Phy-X/PSD.

Energy (MeV)	Effective Atomic Number		
	Auto-Zeff	GRASP	Phy-X
0.01388	64.52	66.17	-
0.01404	64.77	67.73	-
0.01435	65.32	68.96	-
0.015	69.17	69.54	69.54
0.02	69.45	69.92	69.92
0.02435	69.40	67.56	-
0.02551	70.06	66.08	-
0.03	72.69	65.23	65.23
0.04	72.73	65.48	65.48
0.05	72.69	65.71	65.71
0.06	69.95	65.91	65.91
0.07839	47.60	70.85	-
0.08	47.89	66.33	66.33
0.08072	47.83	74.88	-
0.1	67.60	74.78	74.78
0.15	68.05	74.22	74.22
0.2	68.15	73.18	73.18
0.3	67.96	70.64	70.63
0.4	67.49	68.33	68.33
0.5	66.91	66.56	66.56
0.6	66.31	65.27	65.27
0.8	65.21	63.63	63.63
1	64.33	62.70	62.70
1.022	64.27	62.62	-
1.25	63.55	62.04	-
1.5	63.14	61.81	61.81
2	62.87	61.89	61.89
2.044	62.83	61.90	-
3	62.66	62.50	62.50
4	62.58	63.11	63.11
5	62.51	63.61	63.61
6	62.50	64.00	64.00
7	62.47	64.31	64.31
8	62.46	64.56	64.56
9	62.46	64.78	64.78
10	62.46	64.95	64.95
11	62.44	65.10	65.10
12	62.45	65.24	65.24

Table 4.3. (Continued) The effective atomic number for Alloy-A as calculated by Auto-Zeff, GRASP, and Phy-X/PSD.

Energy (MeV)	Effectivve Atomic Number		
	Auto-Zeff	GRASP	Phy-X
13	62.45	65.36	65.36
14	62.46	65.47	65.47
15	62.45	65.55	65.56
16	62.46	65.64	65.64
18	62.49	65.76	65.76
20	62.50	65.86	65.86
22	62.52	65.95	65.94
24	62.52	66.01	66.01
26	62.54	66.07	66.07
28	62.54	66.12	66.12
30	62.55	66.16	66.16
40	62.59	66.30	66.30
50	62.60	66.38	66.37
60	62.61	66.42	66.42
80	62.62	66.47	66.47
100	62.61	66.49	66.49
150	62.59	66.51	66.51
200	62.58	66.52	66.52
300	62.56	66.52	66.52
400	62.55	66.52	66.52
500	62.54	66.52	66.51
600	62.52	66.51	66.51
800	62.51	66.51	66.51
1000	62.51	66.51	66.51

The absorption edges of this sample are located in the range 0.01 – 0.1 MeV. Given the discontinuous nature of cross-section in the vicinity of absorption edges, the effective atomic number must change dramatically there across narrow energy intervals. This is indeed observed while examining the rise and fall of Z_{eff} by GRASP and Auto-Zeff in the table. However, the two do not agree on Z_{eff} in that range of absorption edges 0.01 – 0.1 MeV. The authors of Auto-Zeff acknowledge the uncertainties of their software in these lower regions[3], while the error of GRASP is

[3] Auto-Zeff's uncertainties for high energies (far from the absorption edges) are of the order 1-2%. But for lower energies down to 0.001 MeV, the uncertainty can range up to 25-50% [5].

certainly due to the improvised fitting it performs for the cross-sections near the absorption edges (more in section 3.3.2.). In addition, GRASP does not let Z_{eff} to be multivalued at absorption edges (see section 3.3.3.). Figure 4.2. illustrates these findings graphically, using the data from Table 4.3.

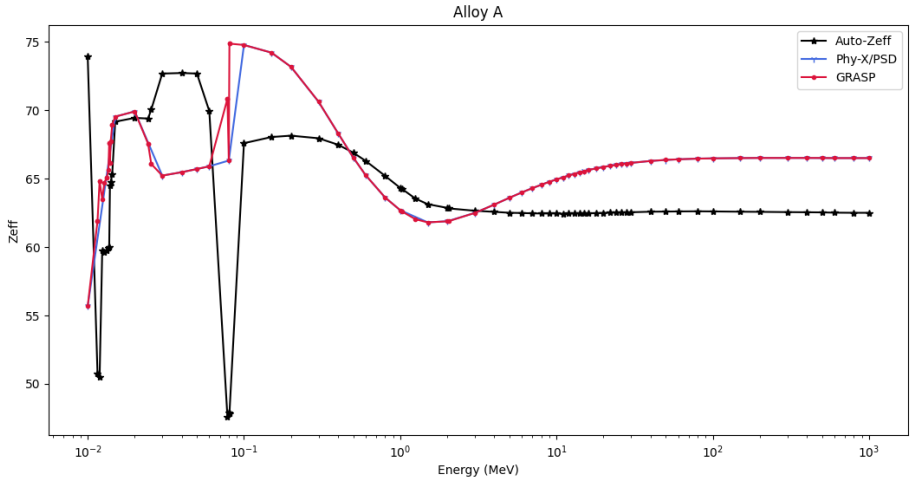

Figure 4.2. Comparison of Zeff as calculated by Auto-Zeff, Phy-X, and GRASP for the casting gold alloy labeled as Alloy-A.

In the region of 0.1 MeV and beyond, in general, GRASP tends to steadily overestimate Z_{eff} in comparison with that of Auto-Zeff, which could be due to the difference in the calculation method. Since Phy-X/PSD also uses the same equation as GRASP, both of them perfectly agree across all the span of standard energies. Phy-X's plotline in Figure 4.2 is represented by a blue line that is barely visible because it is overshadowed by GRASP's red line as they go over the exact same points. Phy-X does not include absorption energies, thus it has less data points in the lower energy region 0.01 – 0.1 MeV, where it can be seen more clearly in the figure.

For the second stage, the sample studied is Acrylic, a coating material also used in dental treatment [34]. This sample is made up of carbon, hydrogen, oxygen, and some nitrogen. The formula is as follows

$$74C_5H_8O_2 + 9C_6H_{10}O_3 + 9C_6H_{10}O_2 + 4C_9H_{13}N + 4C_{14}H_{22}O_6$$

Z_{eff} as a function of energy is calculated for Acrylic in the range 0.01 – 1000 MeV by the three programs. The result is shown graphically in Figure 4.3.

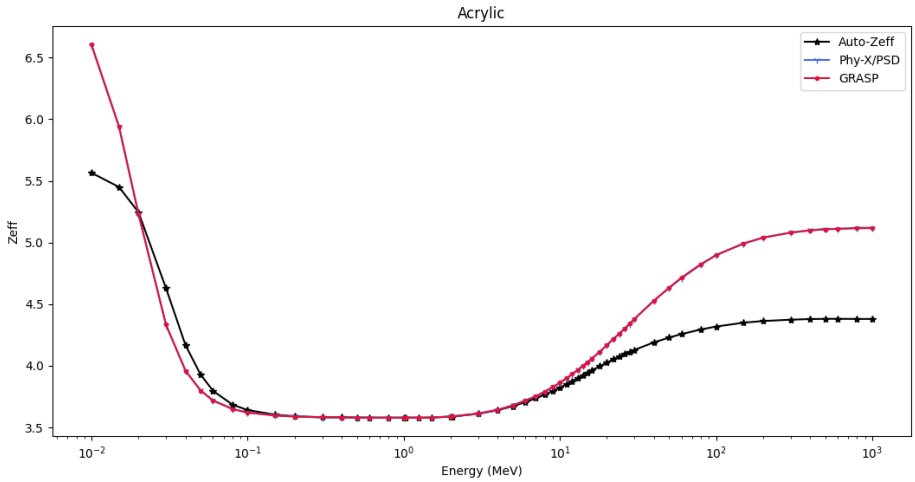

Figure 4.3. Comparison of Zeff as calculated by Auto-Zeff, Phy-X/PSD and GRASP for acrylic.

The plotlines in this figure, are smoother than what was seen from the lower energy regions of Figure 4.2. This is to be expected as there is an absence of absorption edges for the elements constituting this material across this energy range. Again, Phy-X and GRASP produce the same results, which is why they completely overlap. The interesting region of 0.1 – 8 MeV shows all three programs to be in complete agreement for the value of Z_{eff}, which averages about 3.6. It means acrylic behaves roughly between lithium ($Z = 3$) and beryllium ($Z = 4$) in that region. Beyond 8 MeV, however, GRASP and Phy-X overestimate Z_{eff}. Again, this must be attributed to the different approaches of calculating Z_{eff} between Auto-Zeff and the other two.

Generally speaking, the Z_{eff} curves produced by these programs have the same shape roughly, in the sense that they rise and fall, or remain flat, at the same energies. This remark could not be stated for samples containing high Z materials with absorption edges in the range, as demonstrated in Figure 4.2. Nevertheless, it is safe to say that GRASP performs just as good as Phy-X for calculations of Z_{eff} of any material across any range, while it recognizes more data points in the lower energy regions due to absorption edges. In comparison to Auto-Zeff, GRASP tends to overestimate Z_{eff} in higher energy regions, while its exhibited deviation is more chaotic in the lower energy regions. No solid statement can be offered for the middle energy regions; the two programs can agree sometimes if the material is comprised of light elements.

5. CONCLUSION

GRASP, standing for Gamma Ray Attenuation Shielding Parameters, is introduced in this work as a newly developed computer program which calculates various gamma shielding parameters. The program is developed in Python code, and it is compatible with machines with Windows operating system. For any material under investigation, GRASP requests its composition and density as input, in addition to the energy range of interest. With the help of XCOM, the program reads the photon cross section of the elements constituting the material, then it evaluates the mass attenuation coefficients, effective atomic numbers, and other shielding parameters for the mixture or compound being studied. The output displays tables and graphs produced by the program. The accuracy of GRASP has been validated against calculations of other programs for materials available in the literature. Ideas for further work on improving the program may include expanding it with more shielding parameters, developing a GUI or building a dedicated web page for ease of access, enhancing its calculation speed, etc. In its current state, the program is reliable and competent as a tool for the investigation of shielding parameters.

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