4.0 THE THEORY, ANALYSIS AND CALCULATIONS

Tritium activity concentration inside the human body depends upon the excretion or removal rate from the body. The removal rate is dependent upon water intake as well other water exchange processes from the body. Effective half-life of tritium is governed by biological half-life because nuclear half-life is constant. The gamma-ray photon interacts with elements, compounds or mixtures mainly by the photoelectric absorption, Compton scattering and pair production. The photon interaction is defined mainly by mass attenuation coefficients, mass energy-absorption coefficients, effective atomic numbers and effective electron densities. The photon buildup in shielding and dosimetric materials is estimated using the buildup factors. The fast neutron shielding effectiveness is evaluated by macroscopic effective removal cross-section.

4.1 BIOLOGICAL HALF-LIFE OF TRITIUM

Tritium in the body fluid is estimated by bio-assay samples (preferably urine) because tritium attains equilibrium with body fluid i.e. blood, sputum and urine. Since urine analysis is highly accurate, precise, sensitive and of low cost, therefore it is being used for internal dose estimation. The urine samples for tritium activity are analysed using liquid scintillation counting techniques. The scintillation or light flash produced by beta of tritium is detected by two face-to-face or three facing each other photomultiplier tubes which convert light flash to charge and subsequently to current/voltage signal.

Tritium activity A (t) in the body fluid at any time, t after an intake is given by:

\[
\frac{dA}{dt} = -(\lambda_R + \lambda_B)A \tag{4.1}
\]

the solution of above equitation is

\[
A(t) = A_0 \exp(-\lambda_E t) \tag{4.2}
\]

where \(A_0\) is tritium activity taken into the body and \(\lambda_E\) is effective decay constant which is sum of nuclear decay constant, \(\lambda_R\), and biological decay constant, \(\lambda_B\). So effective half-life of tritium is given by following relation:

\[
\tau_B = \frac{\tau_E \times \tau_R}{\tau_E + \tau_R} \tag{4.3}
\]

where \(\tau_E\), \(\tau_B\) and \(\tau_R\) are effective, biological and nuclear half-lives, respectively. The disintegration constant, \(\lambda\) is described as \(\lambda = \frac{0.6932}{\tau}\). Since the nuclear half-life of tritium is known, so using the eq (4.3) the biological half-life can be estimated. The specific activity \(A\) of body water volume (L) after tritium intake is given by:

\[
A(t) = \frac{A_0 \exp(-\lambda_E t)}{L} \tag{4.4}
\]
4.2 COMPUTATION OF GAMMA INTERACTION PARAMETERS

The transmission of gamma-ray photons through a medium is shown in the figure 3.3.7, where mono-energetic collimated narrow gamma-ray photon beam is allowed to hit a detector after passing through an absorbing medium. The intensity of transmitted beam of gamma-ray photon follows exponential attenuation. The gamma-ray photons are being removed either by absorbing or scattering in the medium. The photoelectric absorption, Compton scattering and pair production interaction processes work based on the photon energy and atomic number of the medium. The linear attenuation coefficient application is limited for interaction whereas mass attenuation coefficient is being used due to the fact that the mass attenuation coefficient is constant for an absorber for a particular energy.

4.2.1 MASS ATTENUATION COEFFICIENT AND LINEAR ATTENUATION COEFFICIENT

The mass attenuation coefficient for a compound or mixture is being calculated by the mixture rule\[130\] as:

$$\left( \frac{\mu}{\rho} \right) = \sum_{i} w_i \left( \frac{\mu_i}{\rho_i} \right)$$

where $w_i$ is the proportion by weight and $(\mu/\rho)_i$ is mass attenuation coefficient of the $i^{th}$ element.

The linear attenuation coefficient, $\mu$ is calculated by multiplication of $\mu/\rho$ and the density as given below:

$$\mu = \frac{\mu}{\rho} \times \rho$$

The linear attenuation coefficient is sum of the probabilities per unit length of photoelectric absorption, $\tau$, Compton scattering, $\sigma$ and pair production, $\kappa$ as equation given below;

$$\mu = \tau(\text{photoelectric}) + \sigma(\text{compton}) + \kappa(\text{pair})$$

4.2.2 MEAN FREE PATH

The gamma-ray photon can also be characterised by their mean free path, $\lambda$, defined as average distance travelled in the absorber before an interaction takes place. Its value can be obtained from eq (4.8) below as:

$$\lambda = \frac{\int_{0}^{\infty} x e^{-\mu x} dx}{\int_{0}^{\infty} e^{-\mu x} dx} = \frac{1}{\mu}$$

The mean free path is simple reciprocal of linear attenuation coefficient. The typical values of $\lambda$ range are from few millimeters to tens of centimeter in solid.
4.2.3 MASS ENERGY-ABSORPTION COEFFICIENT

Similar to the mass attenuation coefficient, mass energy-absorption coefficient is defined for absorption of the energy of the gamma-ray photon in the medium. The mass energy-absorption coefficient, \( \mu_{en}/\rho \) for compound or mixture is calculated by following eq (4.9):

\[
(\mu_{en}/\rho) = \sum_{i} w_i (\mu_{en}/\rho)_i \tag{4.9}
\]

where \( w_i \) and \( (\mu_{en}/\rho)_i \) are the proportion by weight and the mass energy-absorption coefficient of the \( i \)th elements present in the compound or mixture.

4.2.4 HALF-VALUE LAYER AND TENTH-VALUE LAYER

Half-value layer (HVL) and tenth value layer (TVL) are the thickness of the absorbing materials which reduces the intensity of incident gamma-ray photon by 1/2 and 1/10th. The HVL and TVL are given as:

\[
HVL = \frac{0.6932}{\mu} \tag{4.10}
\]

and

\[
TVL = \frac{2.303}{\mu} \tag{4.11}
\]

4.2.5 EXPOSURE BUILDUP FACTOR AND ENERGY ABSORPTION BUILDUP FACTOR

The buildup factors of photon in a medium for exposure as well as energy absorption are calculated using Geometric Progression (G-P) fitting method. In brief, the computational work is being divided into three steps;

1. Calculation of equivalent atomic number \[^{[89,131]}\]
2. Calculation of the G-P fitting parameters \[^{[89,131]}\]
3. Calculation of the buildup factors \[^{[105,132]}\]

First of all equivalent atomic number, \( Z_{eq} \) for compounds or mixtures is estimated by ratio of \( (\mu/\rho)_{Compton} \) / \( (\mu/\rho)_{Total} \) at a specific energy with the corresponding of an element at same energy. Thus, firstly the Compton partial mass attenuation coefficient, \( (\mu/\rho)_{Compton} \) and the total mass attenuation coefficients, \( (\mu/\rho)_{Total} \) are obtained for the compounds or mixtures in the energy region 0.015 to 15 MeV using WinXCom program developed by Gerward et al. \[^{[84]}\]. The \( Z_{eq} \) is calculated using logarithmic interpolation by following eq (4.12) as given below:

\[
Z_{eq} = \frac{Z_1 (\log R_2 - \log R) + Z_2 (\log R - \log R_1)}{(\log R_2 - \log R)} \tag{4.12}
\]
where \( Z_1 \) and \( Z_2 \) are the atomic numbers of the elements corresponding to the ratios \( R_1 \) and \( R_2 \) respectively. \( R \) is the ratio, at specific energy lies between two successive ratios of the elements.

Secondly, the G-P fitting parameters are calculated similar to the equivalent atomic number. The G-P fitting parameters for the elements are taken from the ANSI/ANSI-6.4.3, 1991 standard database which provides the G-P fitting parameters for 23 elements (Be, B, C, N, O, Na, Mg, Al, Si, P, S, Ar, K, Ca, Fe, Cu, Mo, Sn, La, Gd, W, Pb and U) in the energy region 0.015 to 15 MeV up to 40 mfp penetration depth. The work in under progress for updating \[^{133, 134, 135}]\) buildup factors of the elements. The G-P fitting parameters for the compounds or mixtures are calculated using logarithmic interpolation by following eq (4.13) as given below:

\[
P = \frac{P_1 (\log Z_2 - \log Z_{eq}) + P_2 (\log Z_{eq} - \log Z_1)}{(\log Z_2 - \log Z_1)} \quad (4.13)
\]

where \( P_1 \) and \( P_2 \) are the values of the G-P fitting parameters corresponding to the atomic numbers of \( Z_1 \) and \( Z_2 \) respectively at a given energy.

Third step is buildup factors estimation by G-P fitting parameters \( b, c, a, X_k \) and \( d \) in the photon energy range of 0.015 to 15 MeV up to a 40 mfp by the following eqs (4.14)- (4.16):

\[
B(E, x) = 1 + \frac{(b - 1)(K^x - 1)}{K - 1} \quad \text{for} \quad K \neq 1 \quad -(4.14)
\]

\[
B(E, x) = 1 + (b - 1)x \quad \text{for} \quad K = 1 \quad -(4.15)
\]

for penetration depth \( \leq 40 \) mfp,

\[
K(E, x) = cx^a + d \frac{\tanh(x / X_k - 2) - \tanh(-2)}{1 - \tanh(-2)} \quad -(4.16)
\]

where \( x \) is the distance from source (in mfp) and \( b \), the value of the buildup factor at 1 mfp and \( K(E, x) \) is the dose multiplicative factor. The variation of \( K(E, x) \) with penetration represents the change in the shape of the spectrum from that at 1 mfp which determined the value of \( b \). The eq (4.16) represents the dependency of \( K \) on \( x \); \( a, c, d \), and \( X_k \) are fitting parameters which depends on the attenuating medium and source energy, \( E \).

### 4.2.6 STANDARISATION OF G-P FITTING METHOD

The G-P fitting method has been compared with ANSI/ANSI-6.4.3, 1991\[^{104}\] and MCNP-5\[^{135}\] for exposure buildup factors in the water\[^{136}\]. The figure 4.2.1 shows that the exposure buildup factors in water by G-P fitting, ANSI/ANSI-6.4.3, 1991 standard and MCNP-5 at different penetration depths are in very good agreement. The MCNP-5 results vary from those ANSI/ANSI-6.4.3, 1991 standards with slightly due to difference in cross-section libraries, method of solution for codes, standard deviation and physics assumptions for bremsstrahlung and coherent scattering\[^{135}\]. The absolute maximum deviation in exposure buildup factors for water are 0.5-3%, 0.9-42.7%, 0.4-53.2% and 0.5-9.3% by G-P fitting, Berger approach, Taylor approach and three-exponential methods\[^{105}\]. Figures 4.2.2 and 4.2.3 show the comparative analysis for exposure buildup factors and energy absorption buildup factors in water for photon for energy 0.015 to 15 MeV at various penetration depths.
Similarly G-P fitting method has been compared with ANSI/ANS-6.4.3, 1991 for lead. Figure 4.2.4 shows the comparative analysis for exposure buildup factors for lead for photon of energy from 0.04 to 15 MeV at various penetration depths. The differences in exposure buildup factors using ANSI/ANS-6.3.4, 1991 and G-P fitting method are within few percentages except near K-edge absorption for lead. This analysis shows that the G-P fitting method is an excellent method for computation of the buildup factors for compounds or mixtures.

Figure 4.2.1: Exposure buildup factors for water obtained from ANSI/ANS-6.4.3, 1991 standard data (line) and MCNP-5 (star) comparison with those of from present work G-P fitting (circle) for energy region 0.015-15 MeV at 1, 5, 10, 25 and 40 mfp

Figure 4.2.2: Difference (%) between ANSI/ANS-6.4.3, 1991 standard data and present G-P fitting work with respect to the calculated values of EBF for water at some penetration depths up to 15 MeV
Figure 4.2.3: Difference (%) between ANSI/ANS-6.4.3, 1991 standard data and present G-P fitting work with respect to the calculated values of EABF for water at some penetration depths up to 15 MeV

Figure 4.2.4: Difference (%) between ANSI/ANS-6.4.3, 1991 standard data and present G-P fitting work with respect to the calculated values of EBF for lead at some penetration depths up to 15 MeV

4.3 DOSE EVALUATION

The dose rate from an isotropic point source is given by following eq (4.17):
\[ D = \frac{S_0 B e^{-\mu x}}{K 4\pi r^2} \]  

where \( D \) is dose rate (unit of dose rate), \( S_0 \) is point source of gamma-ray (photon/s), \( B \) is buildup factor (dimensionless), \( \mu \) is linear attenuation coefficient (length\(^{-1}\)), \( x \) is thickness of shield, \( K \) is conversion factor for gamma-ray to dose rate and \( r \) is distance from source to receptor (unit of length). The attenuation of gamma-ray photon is accomplished by three interaction processes namely photoelectric absorption, Compton scattering and pair production. The photoelectric absorption completely removes the photon, pair production remove and regenerate the photons. However, in Compton scattering process the photon interact with the electrons and loses some part of energy. Therefore, some gamma-ray photons reach to the receptor by penetrating the shield which were counted as lost in the calculation of attenuation coefficient. The concept of buildup factor in dose evaluation is introduced from here.

### 4.4 EFFECTIVE ATOMIC NUMBER AND EFFECTIVE ELECTRON DENSITY

The effective atomic number is dimensionless quantity defined for compounds or mixtures to exhibit the properties of compounds or mixtures similar to the atomic number of elements. Presently various types of methods are being used for effective atomic numbers, which are described below.

#### 4.4.1 AVERAGE ATOMIC NUMBER

The average atomic number is calculated using arithmetic mean of atomic numbers of individual elements using chemical formula as:

\[ <Z> = \frac{1}{n} \sum n_i Z_i \]  

where \( n = \sum n_i \).

This arithmetic mean atomic number provides the single value of atomic number of a compound or mixture.

#### 4.4.2 RATIO METHOD

The total atomic cross-section \( (\sigma_t) \) for compounds or mixtures is obtained from \( \mu_m (=\mu/\rho) \) values using the following eq (4.19):

\[ \sigma_t = \frac{\mu_m M}{N_A} \]
where \( M = \sum_{i} n_i A_i \) is the molecular weight of the compounds or mixtures and \( N_A \) is the Avogadro's number. The effective atomic cross-section \( (\sigma_a) \) is calculated using the following equation:

\[
\sigma_a = \frac{1}{N_A} \sum_{i} f_i A_i \left( \frac{\mu_i}{\rho} \right) \tag{4.20}
\]

The total electronic cross-section \( (\sigma_e) \) is calculated using the following relation:

\[
\sigma_e = \frac{1}{N_A} \sum_{i} \frac{f_i A_i}{Z_i} \left( \frac{\mu_i}{\rho} \right) = \frac{\sigma_a}{Z_{\text{eff}}} \tag{4.21}
\]

where \( f_i = \frac{n_i}{\sum_{i} n_i} \) denotes the fractional abundance of the element \( i \)th with respect to the number of atoms such that \( \sum_{i} f_i = 1 \), \( Z_i \) is the atomic number of \( i \)th element. The effective atomic number of a compound or mixture is given by following eq (4.22) as:

\[
Z_{\text{eff}} = \frac{\sigma_a}{\sigma_e} \tag{4.22}
\]

The effective electron density of a compound or mixture is given by eq (4.23) as:

\[
N_{\text{eff}} = \frac{N_A}{A} Z_{\text{eff}} \sum_{i} n_i \tag{4.23}
\]

### 4.4.3 DIRECT METHOD

The effective atomic number for a compound or mixture can be calculated using practical formula\(^{[137]}\)

\[
Z_{\text{eff,Pr}} = \frac{\sum_{i} f_i A_i \left( \frac{\mu_i}{\rho} \right)}{\sum_{j} f_j A_j \left( \frac{\mu_j}{\rho} \right)_j} \tag{4.24}
\]

where \( f_i \) is molar fraction in the mixture/compound, \( \mu \) is linear attenuation coefficient, \( \rho \) is density, \( \mu/\rho \) is mass attenuation coefficient, \( A \) is atomic weight, \( Z \) is atomic number and the ratio, \( A/Z \), between the atomic mass and the atomic number.

The effective electron density is given by \( N_{\text{eff}} = N_A Z/A \) which is generalized as:

\[
N_{\text{eff,PI}} = N_A \frac{n Z_{\text{eff,PI}}}{\sum_{i} n_i A_i} = N_A \frac{Z_{\text{eff,PI}}}{<A>} \tag{4.25}
\]

where \( n_i \) is the number of atoms of the \( i \)th constituent element, \( n \) is the total number of atoms and \( <A> \) is average atomic mass of a compound or mixture.
4.4.4 INTERPOLATION METHOD

The effective atomic numbers for a compound or mixture are calculated using the following logarithmic interpolation formula as:

\[
Z_{eq} = \frac{Z_1 (\log \sigma_2 - \log \sigma) + Z_2 (\log \sigma - \log \sigma_1)}{(\log \sigma_2 - \log \sigma_1)}
\]  

(4.26)

where \(\sigma_1\) and \(\sigma_2\) are the elemental cross-section in between which the atomic cross-section \(\sigma\) of the material lies and \(Z_1\) and \(Z_2\) are atomic numbers of the elements corresponding to the cross-sections \(\sigma_1\) and \(\sigma_2\), respectively.

4.4.5 POWER LAW

Power law method\(^{[138]}\) is used for calculation of effective atomic numbers of a compound or mixture. The effective atomic number using power law method is calculated by the following eq (4.27):

\[
Z_{eff, PL} = x \sqrt{a_1 Z_1^x + a_2 Z_2^x + \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots
\]

(4.27)

where

\[a = \frac{n_i Z_i}{\sum n_i Z_i}
\]

(4.28)

where \(a_1, a_2, \ldots \) are the fractional contents of electrons belonging to element \(Z_1, Z_2, \ldots \) respectively, \(n_i\) is the number of electrons, in one mole, belonging to each element \(Z_i\). The \(x\) values are in the range 2.94\(^{[138]}\) and 3.5\(^{[139]}\).

Also the effective atomic numbers can be calculated using Auto-Z\(_{eff}\) software\(^{[140]}\) for gamma-ray photon energy 10 keV-1000 MeV. The single value effective atomic number and electron density are calculated using XMuDat software by Nowotny\(^{[141]}\).

4.4.6 AIR-KERMA

The air-Kerma, \(K_a\) of a compound or mixture is derived by ratio of mass energy-absorption coefficients of compound or mixture to air by following eq (4.29):

\[
K_a = \frac{K_{\text{Compound}}}{K_{\text{Air}}} = \frac{(\mu_{en}/\rho)_{\text{Compound}}}{(\mu_{en}/\rho)_{\text{Air}}}
\]

(4.29)

The mass energy-absorption coefficient, \(\mu_{en}/\rho\) of a compound or mixture and air can be computed using eq (4.9). The values of \(\mu_{en}/\rho\) are available in the literature by Hubbell and Seltzer\(^{[80]}\).
4.5 UNCERTAINTIES

The uncertainties in $\mu/p$ values of the elements have been reported by Hubbell\textsuperscript{[142]}. In the Compton scattering region, the estimated uncertainty is found to be about 1% whereas the uncertainty varies for low-Z, medium- and high-Z materials.

For elements hydrogen through oxygen uncertainties are about 1% extend from 100 MeV down to about 30 keV. Below 30 keV the uncertainties are as much as 5 to 10% may be found because of lack of information of photon-effect for low-Z elements, correction to experiments for high-Z impurities and departure of the Compton cross-section from Klein-Nishina theory. Above 100 MeV photon energy, uncertainties in $\mu/p$ values may be 5 to10%.

For elements sodium through copper the uncertainties of 1 to 2% are present at lowenergies (10 keV-1 MeV). At medium energies (1 to 100 MeV) the uncertainties of 2 to 3% are present because of uncertainties in pair production cross-sections. The uncertainties in $\mu/p$ values are estimated to be 1 to 2% beyond 100 MeV.

For elements molybdenum though uranium the uncertainties at low energies (10 keV to 1 MeV) range from 1 to 2% far from an absorption edge to 5 to 10% in the vicinity of an edge. In the range 1 to 100 MeV the uncertainties from pair production estimated are 2 to 3% and 1 to 2% above 100 MeV.

The estimated uncertainties in the gamma-ray photon interaction cross-section data are insignificant for energies above 10 keV. Therefore, these cross-section data are used in shielding, dosimetric, medical, biological, industrial applications.

4.6 REMOVAL CROSS-SECTION FOR FAST NEUTRON

Effective removal cross-section for a compound and homogenous mixture may be approximately calculated using the value of linear removal cross-section, $\Sigma_R$ (cm$^{-1}$) or mass removal cross-section, $\Sigma_R/\rho$ (cm$^2$/g) for various elements of compound or mixture by mixture rule\textsuperscript{[143,128]}. Difference in application of mixture for neutron interaction differs as weight fraction is replaced by partial density and mass attenuation coefficient by neutron removal cross-section. The mass removal cross-section and linear removal cross-sections for a compound or mixture are given as:

$$\Sigma_R / \rho = \sum_i w_i (\Sigma_R / \rho)_i$$

and

$$\Sigma_R = \sum_i \rho_i (\Sigma_R / \rho)_i$$

The values obtained for effective removal cross-section using above equations are accurate within 10% of the experimental values investigated for aluminium, beryllium, graphites, hydrogen, Iron, lead, oxygen, boron carbide, etc\textsuperscript{[6]}. The theoretical and experimental $\Sigma_R/\rho$ values of elements and compounds are given in literature\textsuperscript{[129,144,145,146,147]}. The macroscopic effective removal cross-section for fast neutron of a compound is possible to be calculated using the NXcom software\textsuperscript{[148]}. This eq (4.31) has been used in this report for evaluation of shielding effectiveness of materials for fast neutrons. In this report the fast neutrons are considered which have energy in the range 2-12 MeV and covers majority in the reactor applications.

A number of empirical expressions have been proposed for macroscopic removal cross-section ($\Sigma_R$) using the atomic number, Z and the atomic mass, A of the element. These empirical expressions are taken given by Wood\textsuperscript{[143]}. 

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This is an empirical relation derived from experimental measurements of the fast neutron removal cross-section at 8 MeV. It is to be noted that the removal cross-section may vary with sample thickness and energy. However, the variation should not be very great up to about 5 relaxation lengths and at energies 2–12 MeV.

For a compound or mixture a new term effective atomic weight, $A_{\text{eff}}$, has been defined by Singh and Badiger\footnote{149} as:

$$\sum_{i} \frac{k}{\rho} = 0.21 A^{-0.56} \text{cm}^{2} \text{ g}^{-1}$$

$$\sum_{i} \frac{k}{\rho} = 0.00662 A^{-1/3} + 0.33A^{-2/3} - 0.211A^{-1} \text{cm}^{2} \text{ g}^{-1} \quad (\text{For} \quad A > 12)$$

$$\sum_{i} \frac{k}{\rho} = 0.190Z^{-0.743} \text{cm}^{2} \text{ g}^{-1} \quad (\text{For} \quad Z \leq 8)$$

$$\sum_{i} \frac{k}{\rho} = 0.125Z^{-0.565} \text{cm}^{2} \text{ g}^{-1} \quad (\text{For} \quad Z > 8)$$

The average atomic weight $\langle A \rangle$:

$$\langle A \rangle = \sum_{i} f_{i} A_{i}$$

where $f_{i}$ is molar fraction ($\sum_{i} f_{i} = 1$) and $f_{i}$ is defined as the amount of a constituent $f_{i}$ of $i^{\text{th}}$ element divided by the total amount of all constituents in a mixture $\sum_{i} f_{i} = 1$.

### 4.7 COMPUTATIONAL METHODS

The data on absorption of X-/gamma-ray photons for cross-sections and mass attenuation coefficients for elements and number of compounds or mixtures for engineering and medical applications are available in the literature\footnote{80,142}. Photon cross-sections for compounds or mixtures can be obtained using mixture rule described above. The manual work load was reduced by XCOM program, developed by Berger and Hubbell\footnote{150} for cross-section data for photon energy 1 keV to 100 GeV for elements, compounds and mixtures (Z≤100).

#### 4.7.1 XCOM program

XCOM program provides total cross-sections and attenuation coefficients as well as partial cross-sections for elements. Interaction cross-sections and total attenuation coefficients for compounds or mixtures are obtained as sums of the corresponding quantities for the
elements. Cross-sections for elements in the XCOM pertain to isolated neutral atoms, and do not take into account molecular, solid-state effects and chemical effects which slightly modify the cross-sections, especially in the vicinity of absorption edges. The same cross-section data for elements, compounds and mixtures have been provided by NIST\textsuperscript{[151]}. Soon after XCOM was transformed to Windows operating system by Gerward et al.\textsuperscript{[83,84]} where the cross-section data for photon energy 1 keV to 100 GeV are generated for elements, compounds and mixtures in excel form.

4.7.2 XMuDat program

XMuDat is a program to be used for calculation of various photon interaction coefficients. Each material can be composed of components chosen from the elements and further from a number of compounds and mixtures of dosimetric interest. Data for mass attenuation-, mass energy transfer- and mass energy-absorption coefficients in photon energy the range of 1 keV to 50 MeV can be retrieved. XMuDat computer program is able to produce a single-value effective atomic number and electron density for limited compounds for photon energy upto 50 MeV by Nowotny\textsuperscript{[141]}.

4.7.3 MCNP code

Monte Carlo N-Particle Transport code (MCNP)\textsuperscript{[152]} is a simulation tool to calculate gamma-ray interaction parameters in different types of compounds or mixtures, human organs, tissues and shielding materials. The user can apply for boxes, ellipsoids, cones, etc. and 3D geometry which can be filled with materials of arbitrary composition and density. Point, surface or volume sources of radiation can be defined, from which the mentioned particles are emitted with user specified probability distributions for energy and direction. The code then simulates the particle tracks and interactions with the material; according to probability density distributions. MCNP simulation is source-detector geometry dependent. MCNP simulations for calculation of mass attenuation coefficients for various compounds, mixtures, etc. have been used. Experimental setup design used in laboratory, source-detector, and collimator dimension are given as input for run the MCNP simulation. MCNP simulation is geometry dependent; therefore selection of experimental setup plays a crucial role in output.

4.7.4 Geant4 toolkit

Geant4\textsuperscript{[153]} is a toolkit for simulating the passage of particles through matter. It includes include tracking, geometry, physics models and hits. Physics processes cover a comprehensive range, including electromagnetic, hadronic and optical processes, a large set of long-lived particles, materials and elements. Geant4 is applicable for wide energy range starting 250 eV to the TeV. It has been created exploiting software engineering and object-oriented technology. It has been used in applications in particle physics, nuclear physics, accelerator design, space engineering and medical physics. Geant4 code is widely used for the Monte Carlo simulation of the passage of particles transport through the matter. Geant4 simulation is modeling of the photon attenuation through materials in computer environment gives flexibility and ease of use, instead of performing an experimental determination of interaction parameters.