Chapter 2

Computational Codes

This chapter provides an overview of the various theoretical codes used for the reaction cross-section and shielding analysis, which gives the concordances to experimentally measured data. The nuclear reaction code TALYS-1.95 was used for the study of neutron-induced reaction cross-sections from neutron activation analysis. This code was used with their pre-defined level density parameters for the theoretical calculations. In some cases, an level density parameters were adjusted to get better results. The MCNP, WinXCom, Auto-Z_{eff}, and NXcom software were used for the γ-rays and neutron shielding analysis. Among these, MCNP and WinXCom software were used in the calculation of mass attenuation coefficient for γ-rays, which were further used in the calculation of Effective Atomic Number, Electron Density, Half Value Layers (HVL), Tenth Value Layers (TVL) and Mean Free Path (MFP). The Auto-Z_{eff} software was also used for the Effective Atomic Number and Electron Density calculations, in comparison with the data from a direct method. The software NXcom together with the MCNP was used to study the fast neutron removal cross-section. The interplay between the theoretical predictions with the experimentally measured data for neutron-induced reaction cross-sections and γ-rays and neutron shielding analysis are briefly described in the upcoming chapters 3 and 4, respectively.

Neutron-induced nuclear reaction cross-sections play pivotal role in the safety, risk assessments and for overall safe operation of a nuclear reactor system. An accurate and persistent nuclear data are also of immense importance for developing Generation IV reactors. The theoretical nuclear modular code TALYS-1.95 [1] was developed to interpret the experimental reaction cross-section data. The code is designed with different nuclear density models to perform theoretical calculations and give its predictions. In precise information and brief understanding of γ-rays and neutron interaction with materials is also become crucial. The software WinXCom [2] is developed to calculate X-ray and γ-ray attenuation, Auto-Z_{eff} [3] is for effective atomic number, whereas, NXcom is to find the attenuation coefficients of fast neutrons and γ-rays. The simulation transport code MCNP [4] [1] is designed to track many particles types over broad ranges of energies were used in the shielding analysis. In the present work, the latest version of each software were used to evaluate the experimental data. In this chapter, basic details of simulation code and software analysis are provided.

2.1 TALYS-1.9: A Nuclear Reaction Program

TALYS-1.95 is the latest updated computer package of developed at NRG Petten, the Netherlands, and CEA Bruyères-le-Châtel, France. The code is used for the analysis and prediction of the nuclear reaction data. TALYS-1.95 provides a complete and accurate simulation of nuclear reactions that involves $\gamma, n, p, d, t,^3 He$ and α-particles as projectiles in the energy span of 1 keV - 200 MeV with incorporating target nuclei of mass $\geq$ 12. The objective behind this code is to build a bridge between the theory and experimental measurements which provide us detailed information on the fundamental interaction between particles and nuclei in nuclear physics.

TALYS-1.95 can also be used as a data tool to generate nuclear data for all possible reaction channels either in a default mode or after fine-tuning the adjustable parameters available in the reaction models. Data will be generated at user-defined energy and angle grid, for all the possible reaction channels above the resonance region. Further, these generated data will be stored in the various constructed data libraries, where it can be directly or indirectly used in various fields like conventional and innovative nuclear power reactors (GEN-IV), transmutation of radioactive waste, fusion reactors, accelerator applications, homeland security, medical isotope production, radiotherapy, single-event upsets in microprocessors, oil-well logging, geophysics, and astrophysics [1].

TALYS-1.95 is built with various nuclear reaction models which incorporate compound nucleus, pre-equilibrium, and direct reactions. The nuclear database has been created using Reference Input Parameter Library (RIPL) [5]. The TALYS-

[1] The data from MCNP simulation code have been provided by collaborators (Katovsky and Varmuza)

1.95 user manual [1] provide a concise detail on nuclear reactions and the corresponding models employed by the program.

In TALYS-1.95 the default optical model parameters are obtained by adopting the local and global parameterizations of Koning and Delaroche [6]. Hauser-Feshbach model [7] is used to describe the compound nuclear reaction mechanism and an excitation model developed by Kalbach [8] adopted in obtaining pre-equilibrium contribution. Figure 2.1 gives a structural outline of the nuclear models that are incorporated in TALYS-1.9.

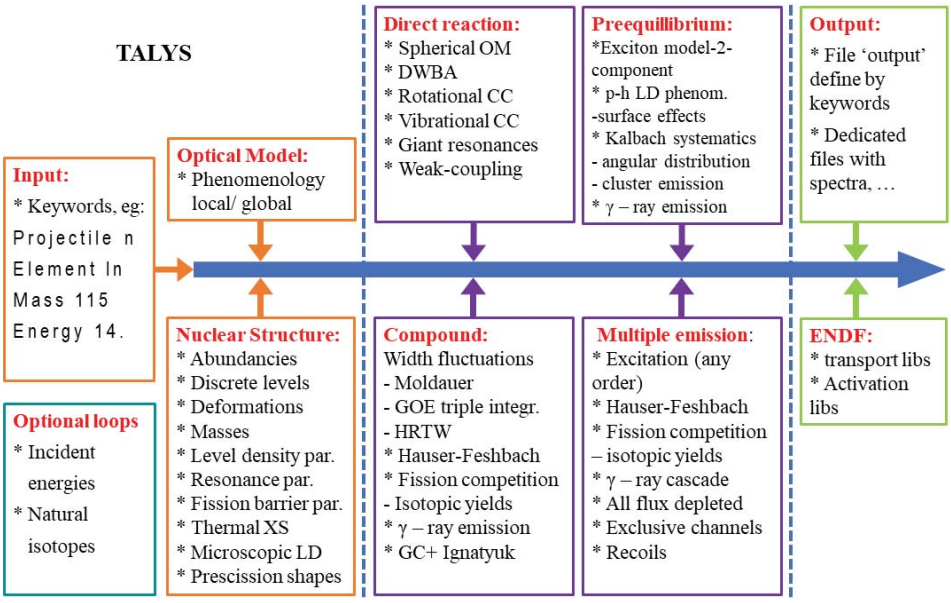

Figure 2.1: A flow chart of nuclear models available in TALYS-1.9 code.

2.1.1 Level Density Models in TALYS-1.95

Six level density models (ldmodel 1-6) [9–14] are available in TALYS-1.95. Among six, three are phenomenological level density models and the rest are for microscopic level densities. These level density models can be simply incorporated in calculation with the help of ***ldmodel 1-6*** keyword and their associated value in the input file of TALYS-1.95

The level density models are listed below:

- **ldmodel 1**: The constant temperature and Fermi gas model [9] (**default**)
- **ldmodel 2**: The Back-shifted Fermi gas model [10]
- **ldmodel 3**: The Generalised superfluid model [11, 12]
- **ldmodel 4**: The Microscopic level densities (Skyrme force) from Goriely's tables [13]

- **ldmodel 5**: The Microscopic level densities (Skyrme force) from Hilaire's combinatorial tables [13]

- **ldmodel 6**: The Microscopic level densities (temprature dependent HFB, Gogny force) from Hilaire's combinatorial tables [14]

TALYS-1.95 also provides a flexibility to adjust level densities [15] and associated parameters. These adjusted parameters other than the default provide more fine-tuning for the experimental data. Basic adjustments can be done by modifying nuclear level density parameter 'a' [15], described below with the presence of shell effects at low energy and their disappearance at high energy in a phenomenological manner.

$$a = a(E_x) = \tilde{a}\Big(1 + \delta W(\frac{1 - e^{(-\gamma U)}}{U})\Big) \tag{2.1}$$

where, U defined as,

$$U = E_x - \triangle \tag{2.2}$$

Here in equation 2.1, $\tilde{a}$ is the asymptotic value of a which would be obtain without considering of shell effects (at $E_x \longrightarrow \infty$), δ W is the shell correction energy. The magnitude of δW determines at low energies showing how a is varied from $\tilde{a}$. The sign of the shell correction term δW varies with respect to $a(E_x)$ whether it increases or decreases as a function of E_x, $\triangle$ is an empirical parameter of the energy shift which incorporated to simulate the odd-even effects in nuclei, the damping parameter γ regulates how briskly $a(E_x)$ approaches to its asymptotic value and can be given as,

$$\gamma = \frac{\gamma_1}{A^{1/3}} + \gamma_2. \tag{2.3}$$

The asymptotic value of a is given by the continuous term,

$$\tilde{a} = \alpha A + \beta A^{2/3} \tag{2.4}$$

In Eqs. 2.3 and 2.4 α, β, and $\gamma_{1,2}$ are global parameters that have been analyzed to give the best average level density description over a whole range of nuclide [1], and A is the mass number. As mentioned earlier in this section, the values of α, β, γ_1, and γ_2 parameters can be adjusted manually in TALYS using **alphald**, **betald**, **gammashell1**, and **gammashell2** keywords, respectively, to find the best fit for the experimental data.

A similar kind of fittings have been applied in present study for $^{113}In(n,n')^{113m}In$, $^{115}In(n,2n)^{114m}In$ and $^{115}In(n,n')^{115m}In$ reaction cross-sections [16], where the data have been fitted perfectly by modifying [2] the value of global parameters α, β

[2]The details are discussed in sections 3.12

and $\gamma_{1,2}$. Whereas default level density model gives the best fit in the study of $^{159}Tb(n,\gamma)^{160}Tb$ [17] and $^{181}Ta(n,2n)^{180}Ta$ [18] reaction cross-sections.

2.2 MCNP: Monte Carlo N-Particle Transport Code

2.2.1 MCNP Overview

The MCNP, is a commonly known **M**onte **C**arlo **N**-**P**article Transport code, developed and maintained by Los Alamos National Laboratory (LANL). The code mainly transports neutrons, γ-rays, and coupled transport, i.e. production of secondary γ-rays generate from neutron interactions, neutron/photon/electron, photon/electron, or electron/photon. The code can be also used to transport primary source electrons and secondary electrons generated through γ-ray interaction. The code allows neutron energy from 10^{-11} MeV to 150 MeV, the proton allows in the energy range 1 keV to 100 GeV, and the electron energy ranges from 1 keV to 1 GeV [19].

2.2.2 General Monte Carlo Approach

Monte Carlo helps solve complex problems, like the nuclear interaction of a particle with materials. It is recreating a statistical process computationally, usually difficult to model in computer codes from deterministic methods. In Monte Carlo method, all the probabilistic events associated with a process are simulated sequentially [19], the whole problem defines in such a manner that these events probability distributions are statistically relying on the choice of random numbers. Figure 2.2 gives an example of a particle interaction history for a neutron imparted on a slab of materials that can undergo fission.

MCNP arbitrarily symbolized between 0 and 1 to determine events either it will follow physics (rules) or transported data (probability) associated with the nuclear process and material used. As the above Figure represented, the collision occurs at event 1 from the imparted neutron. At event 1 physical scattering distribution of the material randomly directed the scattered neutron. A photon is produced and traveled at event 7, for a time it is stored, or banked, for later analysis. Fission occurs of a scattered neutron at event 2, which results in the termination of the scattered incoming neutron and creates one photon and two neutrons. At event 3, among two, the first fission neutron is absorbed and terminated. Left one neutron and photon are stored for later analysis. At event 4, the stored neutron is re-fetch for analysis and through random sampling is examined to leak out of the slab. The stored photon produced from fission is examined, shows a collision at event 5 and escape out at event 6. The photon created from the incident neutron at event 1 goes through at a capture at event 7. Here in the Figure all seven events producing from one particle history. As more and more histories are performed, the distribution nearby reaches the actual [19].

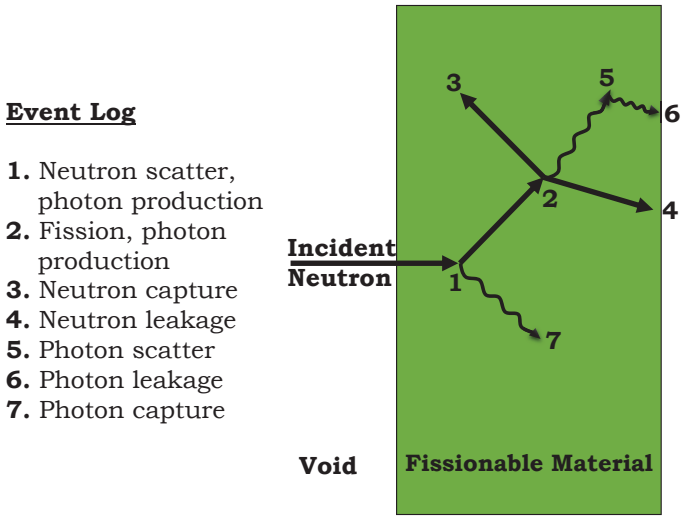

Figure 2.2: Events occurs from the neutron interact history.

2.3 Introduction to MCNP features

Diversify features, concepts, and capabilities of MCNP are encapsulate in upcoming sections. The MCNP has versatile features which help users in many ways, such as designing sources, various geometry plotters, different techniques to minimize variance, and an enriched database of cross-sections.

2.3.1 Structure of Input File

The users can feed the input to MCNP in various forms like the code package, generated by problem runs, or user-supplied. This section gives an idea of the user-created input file, which describes the problem to be run. The input text file that is read by MCNP contains information on the problem including their geometry dimensions, brief details about the material composition, cross-section data libraries, characteristics of the source and its position, the expected outcome-oriented desired tallies, and suitable variance-reduction techniques for better precision [4].

An MCNP input structure has the following form:

A program design in such a manner that command mnemonics in the first five columns and each line contain a maximum of 128 columns and commands. Here, we present only the specific details of the cards required to run the problem. Details about various other commands and errors are given in the user manual [4].

The Figure 2.3 shows the flow chart of the MCNP code. The first line (see fig 2.3) of the MCNP input file is optional but it gives an idea to others which problem is considered and the important points used. Similarly the other cards

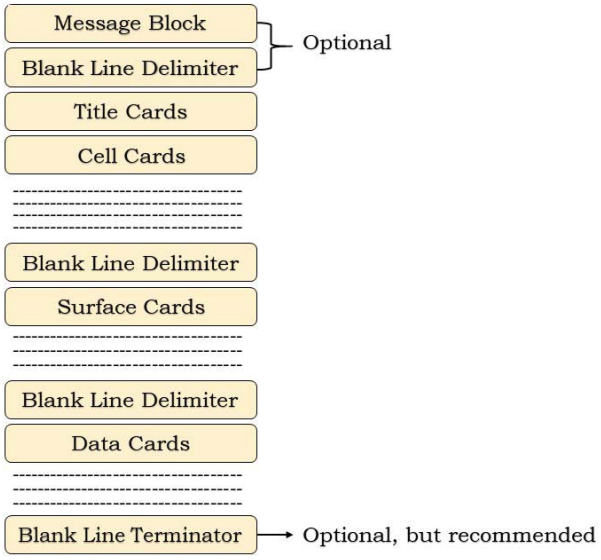

Figure 2.3: Flow chart of MCNP code.

required for the code input are also listed in Figure.

2.4 Geometry Specification

The geometry setup in MCNP can be composed of cell and surface cards. Generally, geometry is considered in point of either regions or volumes covered by 1^{st} and 2^{nd} degree surfaces. Cells are created with the help of intersections, unions, and complements of the regions along with the user-defined materials and density. Geometry defines in terms of 3 dimensional (x, y, z) (cm) Cartesian coordinate system.

All space is composed of contiguous volumes or cells. Each cell is bounded by a surface, multiple surfaces, or by infinity. For example, a cube is bounded by six planes. Every (x, y, z) point must belong to a cell (or be on the surface of a cell). There can be no "gaps" in the geometry, i.e., there can be no points that belong to no cell or surface. Every cell and surface is given by the user a unique numerical identifier.

2.4.1 Cell Cards

In MCNP input cell cards begin with the cell number, immediately after that followed by a material number, which is filled by the user in a particular cell. For that, the user has to define a material with the given same material number in the material card (see section 2.4.8). In case if the cell is void, a zero is assigned for material number, and no density is given for it. The maximum eight-digit numbers allow for both cell and material numbers. The next number that follows

the material number is material density. The user has to chose for the material density, a positive entry is illustrated as atom density of material in units of 10^{24} atoms/cm^3. Where a negative entry is illustrated as mass density in units of g/cm^3. After the material information, proper details are given for the geometry of the cell. This information contains a detail of the assigned surfaces enclosing the cell, each surface denoted with a sign which indicates its regions. The region merges with the boolean intersection and union operators. A space defines an intersection, and a colon (:) indicates a union. After defining the geometry the user can define cell parameters by entering **KEYWORD=value** which is optional.

2.4.2 Surface Cards

Similar to cell cards, surface cards entry starts with a surface number, which begins in one to five columns and limits up to eight digits. Immediate after the surface number user have to assign an alphabetic numeric entry that describes the surface type. The type of a surface is then followed by the numerical card entries sequentially related to the equation of the surface. A detailed description about the mnemonic, type, description, equation, and card entries of surfaces are given in MCNP-primer [20].

2.4.3 Data Cards

The MCNP data input follows the second blank card without message block or the third blank card with message block. The data cards begin with the card name in the first five columns. The necessary entries follow and define after one or more blanks. Mainly block defines the type of particles, suitable materials, type of radiation source, tally specification in which outcomes are stored, type of physics which considered during particle interactions, variance reduction techniques to minimize the error, data libraries of cross-section, the amount and type of output, and different other. More or less, these data cards contain all the information of the problem except the geometry [4].

2.4.4 Mode Card

This card begins with the MODE after being separated by space followed by a particle list use in the transportation. By default, the program considered MODE N (i.e., neutron transport only), if the user omits this card. This card is helping regarding the type of particle that is going to be tracked in the problem [20].

2.4.5 Cell and Surface Parameter Cards

In the input file, the user entered data to particular cells from two dferent cards either on the cell card itself or in the data card section. But for the individual surfaces, the data card format is the only way to entered the data. Here the

number of data entries on this cell must equal the number of cells or surfaces of the problem. If both these do not match MCNP shows a warning or fatal error message. Although the program allows to continue with the assumption that each cell or surface value is zero [20].

2.4.6 Source Specification Cards

This is one of the important cards in the MCNP code, which defines the source and type of radiation particles. Among the four available methods a source definition card SDEF is largely used in defining starting particles. This single command (SDEF) has the capability of generating an vast variety of sources. Mainly variables in the SDEF line can be characterized in three types; explicitly, with a distribution number, and as a function of a new variable.

The second and third type of variables requires three other source cards: the source information (SI) card, the source probability (SP) card, and the source bias (SB) card.

2.4.7 Tally Specification Cards

The tally cards are used to instruct the MCNP code about what you get after the Monte Carlo Calculation. The code has seven different standard types of tallies. The most frequently used tallies are current on a surface (F1), average flux on a surface (F2), particle range estimate of cell flux (F4), particle flux at a point (F5a: N or F5a: P). Similar to flux tallies few tallies are for particle range energy estimate of deposition (F6) and particle range estimation for fission energy deposition (F7: N). For pulses generation in a detector from particle energy distribution (F8). Except this standard tallies code have many optional commands which are briefly described in section 3.3.5 of MCNP Theory Manual [4]. The frequently used tally commands that modify tallies are the En card change into energy bins, the FMn card tally multiplication by some quantity, and the DEn and DFn cards multiply each tally by a fluence-to-response conversion factor. The users can also use a function of tally normalization to single-source particle except for few tallies F6 and F7. At the beginning of the tally, the user adds an asterisk (like, *F1: P) to normalize it, which resulting in tallies of energy flux or energy current. The tally cards are not necessary, but if the user is not specified, tallies will be printed and output displays with a warning message.

2.4.8 Materials Specification Cards

The card contains specifications about the materials used in various cells in the MCNP calculation. In this section, the user define the materials in two way compositions, namely, in terms of isotopes and cross section evaluations that has to be used in the cells. The user has to define a unique material number, the elemental or isotopic composition of corresponding material and the cross-section

compilation have to be used. The density of the material is not provided in this section. Rather, it is specified in the cell card. This benefits the users in that they can include the same material with different densities in various cells.

Mainly two methods are available for material specification, inserting the nuclide fractions it either normalized to one or remain un-normalized and identification number (ZAID) used to define the constituent element or nuclide desired. This number is described in the form of *ZZZAAA.abx*, where *ZZZ* is the atomic number of the element; *AAA* is the atomic mass number of the nuclide except for γ-rays and electrons, the cross-section evaluation specifier is given by *ab* and *x* is the data class. Few commonly used classes are continues energy neutron *C*, *P* is photon, *E* is electron, *U* is photo-nuclear, and *H* is proton. In the case of natural materials, the value of AAA is 000. If the user is omitted the *.abx* then the program selects the first entry from the xsdir relative to the specific library class that will be used. The code used the same approach for all libraries which are undefined [20].

The VOID card is also vastly used in checking the geometry description, basically very effective in finding errors due to its short running time. Due to this card materials used in the problems are removed and fixed all non-zero importance to unity. If the geometry runs with a large number of particles and geometry was not correctly define then the particle getting lost in such area of geometry. This history of lost particles indicates to the users about geometry error. finally, when the user is satisfied with the running report i.e. the geometry is error-free, replace the VOID card with material cards and make a run with the actual parameters. A comprehensive discussion of materials specification is given in section 3.3.2 of MCNP manual [4]. The cards used in the present work are given in the section 4.6.2 of chapter 4.

2.5 WinXCom: X-ray attenuation coefficients program

A γ-ray scattering and absorption data are highly required in applications like scientific, engineering and medical, etc. Previously various authors [21–30] provided cross-sections tables for many elements, but they can considered only few elements. Also, they have provided limited γ-ray cross-section data of compounds and mixtures. Moreover, except [23–30] tables the other contains data for a limited number of compounds and mixtures. However, the materials for which γ-ray cross-sections data are required in various applications are large.

Near the absorption edges, γ-ray cross-section data for compounds obtained as weighted sums of the atomic constituents. However, the numerical work for this procedure is quite tedious, and becomes more complicated when photo-absorption cross-sections and total attenuation coefficients are discontinuous at absorption edges [2]. Hence, the compound cross-section data requires much more additional interpolation. Therefore, a convenient and alternative approach

is required to generate the data for compounds and mixtures. The article of Berger et al., [2] describes a web program known as XCOM which simplifies work for any periodic element, compound, or mixture, in between the energy range of 1 keV and 100 GeV.

In this energy range, the XCOM program generates cross-sections on a logarithmic spaced standard energy grid or a grid preferred by the user, or a combination of both grids. Although, this program automatically includes data of cross-sections at energies promptly above and below all absorption edges.

The basic parameters used in transport calculations and details about the comprehensive database for all elements over a wide range of energies constructed through various publications in [2]

Here in the WinXcom program, the incoherent and coherent scattering cross-section and the total attenuation coefficients are generated through log-log cubic-spline fits as a function of energy. Where the pair-production cross-sections, derived by fitting the logarithm of term $(1 - E/E')^3\sigma_{PAIR}(E)$, where E is the photon energy, E' is the minimum energy required for pair production, and $\sigma_{PAIR(E)}$ is the cross-section. As the E' values are different for both the nuclear (E' = 1.022 MeV) and atomic electrons (E' = 2.044 MeV) field fitting was done individually for pair production. Similarly, at energies above k-shell absorption edge the overall photoelectric absorption cross-section for all shells interpolated in the same manner as in pair production (i.e. log-log cubic-spline fits). Below the absorption edge, changes are governed to the logarithm of the photoelectric cross-section for an individual shell, fitted linearly with the logarithmic function of the photon energy. Here the separate fitting is taken into consideration for each shell which ignores the error that occurred through interpolation near the absorption edges and provides satisfactory fits [2]. The execution of this code for the present work is briefly described in section 4.6.1 of chapter 4.

2.6 NXcom: Fast neutrons and γ-rays attenuation coefficients program

NXcom computer program has been developed for the prediction of removal and attenuation coefficients for neutrons and γ-rays, respectively. The program was developed using version 77 of FORmula TRANslation programming language (FORTRAN77). Similar to WinXcom software, the database of this software incorporates all quantities of partial coefficients (photoelectric absorption, coherent and incoherent scattering, and pair production). With the help of this database, the NXcom software calculates previously stated coefficient for any mixture, compound, and material. The Nxcom software contains two different database files for calculations; the first is for the fast neutrons removal coefficients and the other is for the γ-ray attenuation coefficients.

The outcomes from this software generate into three separate files. The

software's first output file, allotted for fast neutrons attenuation, shows the elemental composition of the inserted mixture, compound, or material, listed in ascending order considering the atomic numbers, along with the fraction by weight of the constituents, mass removal cross-section, partial density and the macroscopic neutron removal cross-section of the investigated material. Whereas the second file contains the same data information for all compounds added along with the investigated mixture or material. The third output file contains the data regarding the attenuation of γ-rays. Here, the output files give the cross-sections and attenuation coefficient on a standard energy grid of the Xcom program, except at the absorption edges. For mixture, compounds, and materials the program provides the interaction coefficients and total attenuation coefficients as a sum of the quantities for the elemental constituents. Only the user has to enter either the chemical formula (compound) or the fractions by weight of the components (mixtures) into the program, which itself calculate weighting factor and start the calculation of the various coefficient. The main advantage is that this program required only one input file for calculations of both removal and attenuation coefficients of fast neutrons and γrays, respectively [31].

2.7 Auto-Z_{eff}: Calculation of effective atomic numbers program

As all, we know the atomic number Z has a strong connection with the fundamental properties of the elements. Similarly, effective atomic number Z_{eff} is necessitates for composite or mixture. Previously, the method of evaluating effective atomic number Z_{eff} required quite laborious calculation, to overcome this many researchers and scientists turn back to the most common and simplistic power-law methods [3]. They used power law in the form:

$$Z_{eff} = \sqrt[m]{\sum f_i Z_i^m} \tag{2.5}$$

where f_i is the relative electron fraction i^{th} element Z_i, in a way that $\sum f_i = 1$. For the exponent m value 2.94 suggested by Mayneord [32], this can be found in basic radio therapy books [33].

2.7.1 About Auto-Z_{eff} program

The Auto-Z_{eff} program was developed and compiled within the Microsoft Visual Studio 2010 development suite (Version 10.0.30319.1) using the Microsoft Visual Basic.NET programming language.

The program contains precalculated data files for the first 100 periodic elements, with mass attenuation coefficients and cross-section matrices as a function of photon energy. It also loads the predefined material files and photon source spectra. The user either selects these predefined materials or creates

a new material from user-defined material with the help of elements and their fractional components. At later, whenever a user wants they use these predefined material files. Not only that, but the program also allows to load source spectra files in a user-defined section. The program allows Z_{eff} calculation for user-defined material after confirming that the fractional sum of user define material is 1.0. Once the material-defined program quickly starts the Z_{eff} calculation. At beginning of the calculation, first, it selects the mass attenuation coefficient data files for each element included in the selected materials. The total attenuation coefficient is calculated through liner additivity at the energy grid included in the mass attenuation coefficient data files, based on the mass fraction of each element of the material. Further, the cross-section for each energy is calculated. The final effective atomic number is determined with the help of this calculated cross-section and lookup table of preloaded cross-section matrix for each element. Before the determined effective atomic number data is displayed the program compares the calculated cross-section relative to the cross-section matrix data via interpolation at each energy. This calculated effective atomic number data are displayed graphically in the Z_{eff} (E) tab along with the exportable table [3].

The program also evaluates the effective atomic number at user-specified single-valued using Eq. 2.6, where Ψ(E) is the energy spectrum (normalized to unity):

$$Z_{eff} = \sum_i Z_{eff}(E_i)\Psi(E_i) \cong \int_{E_{min}}^{E_{max}} Z_{eff}(E)\Psi(E)\,dE \tag{2.6}$$

2.7.2 Functionality of the Auto-Z_{eff} program

A detailed procedure to run the Auto-Z_{eff} program is illustrated in this section. Firstly, whenever the user opens this program it starts with loading splash screen. After the disappearing splash screen, the program will step into the material definition, in which the user has specified the material from a list of predefined or user-defined sections. The predefined or user-specified material selection screen shown in Figure 2.4. As per shown in Figure 2.5 the program analysis to ensure that the fractions sum of the user define inserted material is unity and the medium is defined. After this ensuring the sum and medium was defined, effective atomic number are calculated relative to energy in the spectrum range of 10 keV to 1 GeV, as shown in Figure 2.6. Rather than this entire energy spanning of 10 keV to 1 GeV, the user can also calculate effective atomic number at single-valued or relevant to a particular application. As given in Figure 2.7 the user chooses from a list of predefined spectra (for radioisotopes corresponding to nuclear medicine, Cobalt therapy, kilo-volt treatment, and diagnostic devices, and megavolt radiotherapy devices) or insert their spectrum of interest. This then allows calculation at a user-defined, spectrum-weighted effective atomic number [3]. In shielding analysis, the MCNP code has been used as the main tool for the theoretical calculations. In addition to MCNP, XCOM, Auto-Z_{eff} and

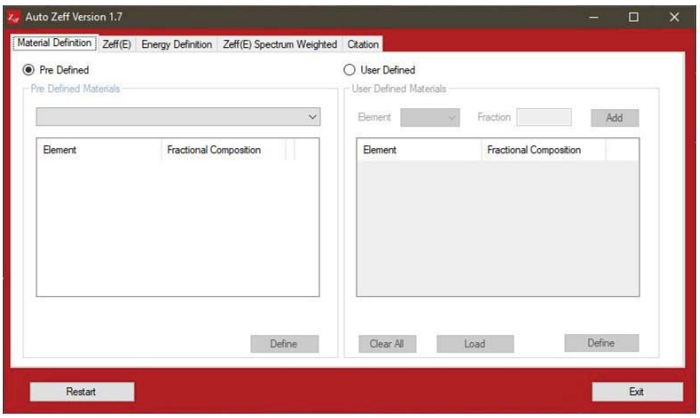

Figure 2.4: Program allows predefined or user-specified media.

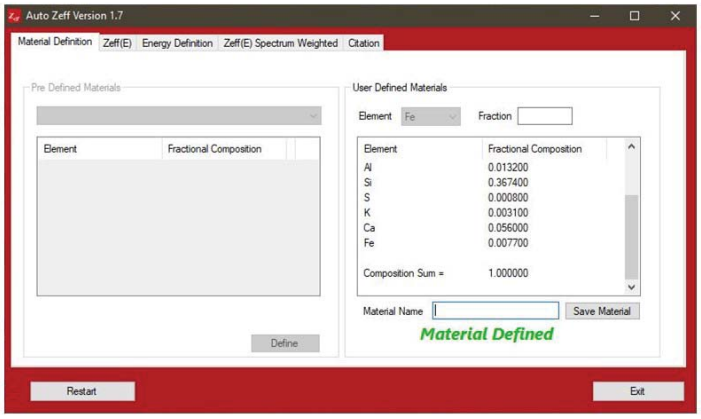

Figure 2.5: The program checks to ensure the fractions sum to unity.

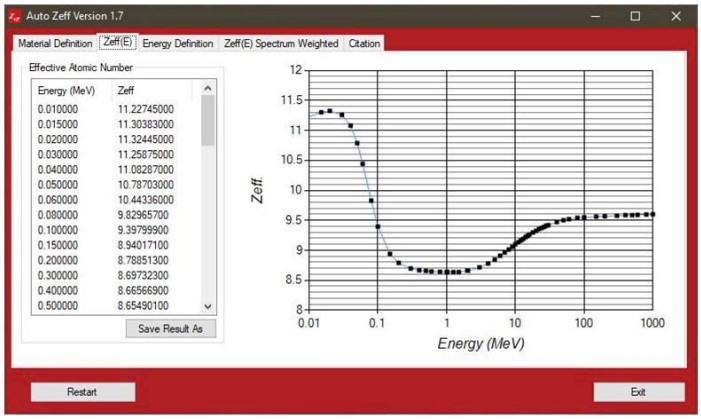

Figure 2.6: Generate Z_{eff} as a function of energy.

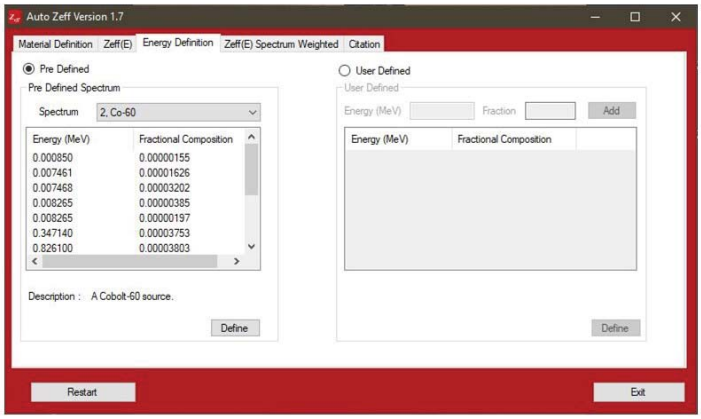

Figure 2.7: Elect a predefined spectrum or insert a single valued energy of interest.

NXcom were used for the comparison and validation of the theoretical codes themselves. The purpose of the comparison was to check and validate the results of different codes using similar input data. This would be helpful for other users to build confidence and reliability over XCOM, Auto-Z_{eff} and NXcom for the prediction of shielding parameters.

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