Chapter 4

Theoretical Nuclear Model Codes

In the present chapter, a brief insight is provided into the theoretical model calculations and the parameters which are used for the optimization of the measured data. The flow of the calculations are also summarized briefly. Three nuclear model codes, TALYS-1.9, EMPIRE-3.2.3-Malta and ALICE-2014, were extensively used with their available input level density parameters for the theoretical calculations. The TALYS-1.9 and EMPIRE-3.2.3-Malta codes were used mainly for the neutrons activation analysis and ALICE-2014 together with TALYS-1.9 was used for the proton induced reaction cross-section data. The comparison of the theoretical results with the measured data are shown in the chapters 5 and 6, for neutron and proton induced reactions, respectively.

An important aspect of the study of γ, n, light and heavy-ion induced nuclear reactions is to understand and provide a better explanation for the different processes that take place when a highly energetic projectile hits the target nucleus. The experimental data and the physical interpretations thus achieved enable us to develop different nuclear models for various interaction mechanism. Nuclear model codes like, TALYS [1], EMPIRE [3], ALICE [4, 5] and many more, were developed to understand the nature of experimental reaction cross-section data. Each of these codes may contain different nuclear reaction models, based on which, the code performs theoretical calculations and provide its predictions. Therefore, the experimental data may lead to more refined codes which in future can be used to predict the nuclear data more precisely. In the present work, we have used the latest versions of the above three nuclear model codes, depending upon the applicability based on the chosen nuclear reaction. Each code is equipped with different nuclear models which can be controlled by specific input keywords. A brief discussion about the nuclear reactions has been provided in the section 1.5 and the basic details, model description, flow of calculations and the overview of these codes for present work are describe in the following sections of this chapter.

4.1 TALYS-1.9 Model Code

TALYS is a computer package which is widely used for the analysis and prediction of the nuclear reaction data. TALYS simulates the nuclear reactions that involve γ, n, p, d, t, $^3He-$ and α-particles, within the energy region of 1 keV - 200 MeV. The target nuclei mass may be taken as $\geq$ 12. The primary purpose of TALYS is to play key role in between the theory and experiments which enable us to look into the fundamental interaction between different projectile & target combinations. The understanding on fundamental level result in different nuclear models, which help in return to predict the nuclear reaction data at a given parameter. TALYS can also be used as a tool to describe the available data with the adjustable parameters of different models present in it. TALYS has been used over the years for the prediction of the reaction data related to 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 is equipped with different nuclear reaction models which comprises compound nucleus, pre-equilibrium and the direct reactions. The

input reaction parameters are being taken from the Reference Input Parameter Library (RIPL) [2]. The optical model parameters are obtained by using a global potential proposed by Koning and Delaroche [6]. The compound nucleus reaction mechanism is integrated by using the Hauser-Feshbach model [7] and the pre-equilibrium contribution is calculated by using an exciton model developed by Kalbach [8]. A flow-chart of the TALYS calculations is shown in Figure 4.1

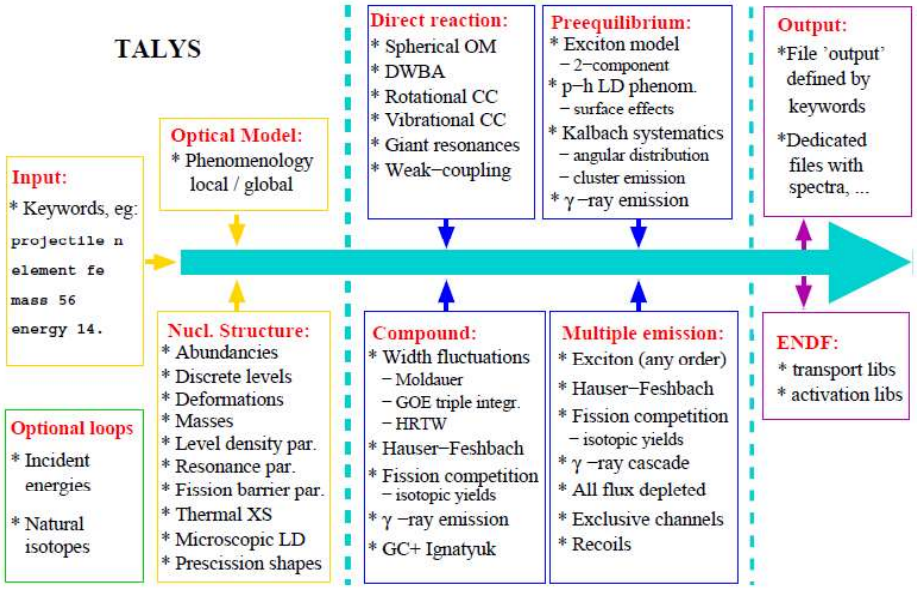

Figure 4.1: A flow chart representation of the TALYS model calculations.

4.1.1 Level density models in TALYS-1.9

TALYS-1.9 [1] has six level density models [9–14], which can be used to predict and to compare different nuclear reaction data appropriately. These level density models can be invoked by using *ldmodel 1-6* keyword in the input description of the code. The level density models are:

- ldmodel 1: Constant temperature + Fermi gas model [9] (default)
- ldmodel 2: Back-shifted Fermi gas model [10]
- ldmodel 3: Generalised superfluid model [11, 12]
- ldmodel 4: Microscopic level densities (Skyrme force) from Goriely's tables [13]
- ldmodel 5: Microscopic level densities (Skyrme force) from Hilaire's combinatorial tables [13]

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

In general the level density parameter [15] can also be adjusted, to fine tune the fitting for the experimental data, by directly changing the values of certain parameters in the level density parameter (a) [15], which is given as,

$$a = \tilde{a}\Big(1 + \delta\epsilon_0\big(\frac{1 - e^{-\gamma U}}{U}\big)\Big) \tag{4.1}$$

with U defined as,

$$U = E_x - \triangle \tag{4.2}$$

where, $\tilde{a}$ is the asymptotic value of a at high excitation energy (E_x), $\delta\epsilon_0$ is the shell correction of the nuclear binding energy, whose magnitude establishes how a is different from $\tilde{a}$ at low energies. The sign of the shell correction term $\delta\epsilon_0$ regulates whether $a(U)$ increases or decreases as a function of effective excitation energy U, $\triangle$ is the energy shift which is included to simulate the odd-even effects in nuclei, γ is the damping parameter, which governs how fast λ approaches $\tilde{a}$ and can be given as, $\gamma = \frac{\gamma_1}{A^{1/3}} + \gamma_2$. The level-density parameter shows the presence of shell effects at low energies and their disappearance at high energy in a phenomenological manner. The asymptotic value of $\tilde{a}$ is given by,

$$\tilde{a} = \alpha A + \beta A^{2/3} \tag{4.3}$$

where A is the mass number, α, β and $\gamma_{1,2}$ are global parameters that have been determined to give the best average level density description over a whole range of nuclide [1]. The values of α, β, γ_1 and γ_2 can be adjusted in order to find suitable fit for the experimental data. A similar kind of attempts have been made in our study of $^{232}Th(n,\gamma)$ and $^{100}Mo(n,2n)$ reaction cross-sections [16,22], where the data have been fitted perfectly by modifying[1] the value of global parameters α, β and $\gamma_{1,2}$.

4.1.2 Pre-equilibrium models in TALYS-1.9

There are different PE models incorporated in TALYS-1.9 [1], to provide a better description of the data for the nuclear reactions involving a major contribution from PE emission. The basic description for the PE calculations are taken from the well known exciton model [18–20] for two-body systems. It is assumed that the total excitation energy E_{Tot} can be distributed among the excitons ($n = p + n$, where p stands for particles and n for holes below

[1]The details are discussed in sections 5.7.1 and 5.8.1

the Fermi surface E_f) has equal probability. The number of ways in which different excitons may share the excitation energy is equal to n. A flow of the equilibrium process for an excited nucleus is shown in Figure 4.2. There

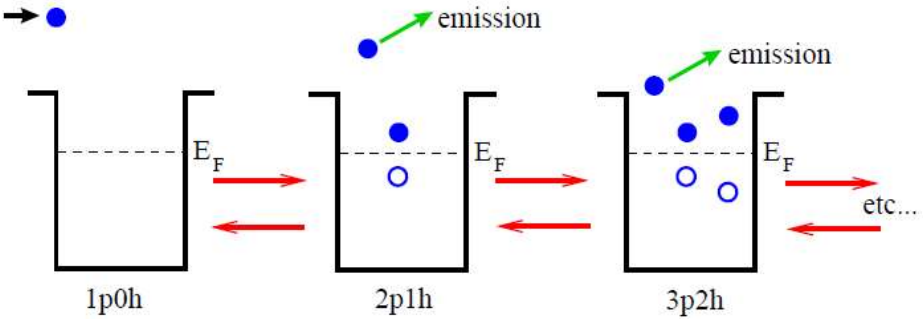

Figure 4.2: Reaction flow of PE equilibrium in Exciton Model [1, 18].

are two versions of exciton models have been incorporated in TALYS-1.9; first is the default two-component exciton model [20] and the second is the one-component exciton model [19]. Four different combinations of PE models can be invoked by using the *preeqmode 1-4* keyword in the input file of the TALYS-1.9 [1] according to the user's need, which are;

- preeqmode 1: Exciton model: Analytical transition rates with energy-dependent matrix element.
- preeqmode 2: Exciton model: Numerical transition rates with energy-dependent matrix element. (default)
- preeqmode 3: Exciton model: Numerical transition rates with optical model for collision probability.
- preeqmode 4: Multi-step direct/compound model.

In the present work, the PE modes have been tested to fit the experimental data and to calculate the PE fraction[2] for the proton-induced reactions.

4.2 EMPIRE-3.2.3-Malta Nuclear model Code

EMPIRE is another nuclear model code package comprising of different codes developed by authors around the globe [3]. The code can perform a number of calculations in a wide energy range up to few hundred MeV. The incident particles can be chosen as γ, n, p, d, t, ^3He, α's and other light or heavy-ions. Major reaction models such as; optical model, Coupled Channels and DWBA (ECIS06 and OPTMAN) [21–25], Multi-step

[2]See section 6.5

Direct (ORION + TRISTAN) [26], NVWY Multi-Step Compound [27] are included. The pre-equilibrium process is being incorporated by using phenomenological models like; exciton model (PCROSS) [28], hybrid Monte Carlo simulation (DDHMS) [29]. The compund nucleus contribution taken care by a full featured Hauser-Feshbach model [30–32] including width fluctuations and fission is calculated by the optical model. The heavy-ion fusion cross section can be calculated by using a simplified coupled channel approach (CCFUS) [33]. The input parameters are taken from the RIPL-3 library [2], which covers nuclear masses, optical model parameters, ground state deformations, discrete levels and decay schemes, level densities, fission barriers, and γ-ray strength functions. EMPIRE can also be used for the calculations of the prompt fission neutron spectra (PFNS), plotting of PFNS, $\bar{\mu}$, and $\bar{\nu}$, anisotropic angular distributions for compound elastic and inelastics, simulation of the Engelbrecht-Weidenmuller transformation [34], and new I/O subroutines for manipulating the ENDF-6 formatted files. Covariance can also be generated within the EMPIRE module by using the KALMAN script[3]. A flow chart for the EMPIRE calculations is shown in Figure 4.3 using the input and output parameters. In the present work, the

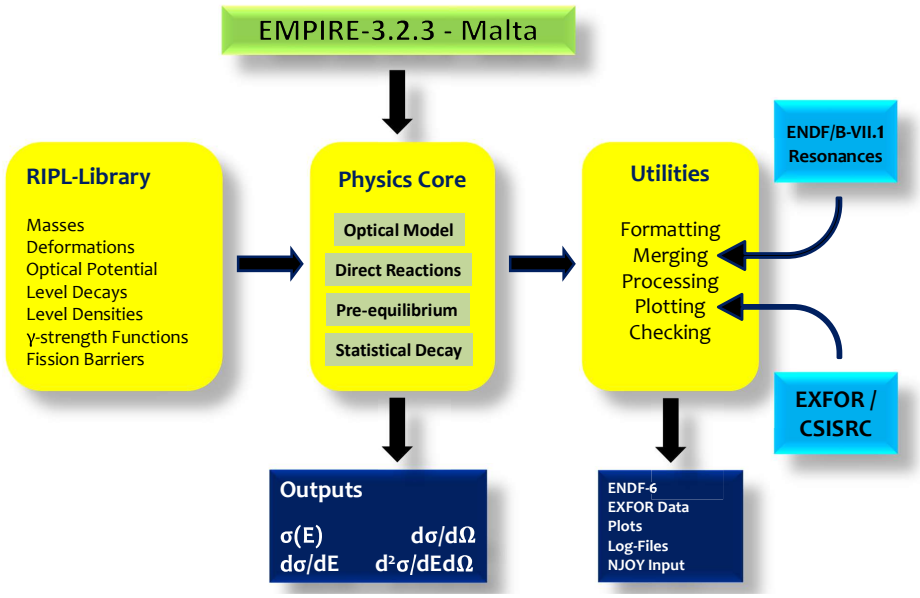

Figure 4.3: A flow chart representation of the EMPIRE-3.2.3-Malta calculations [3].

EMPIRE-3.2.3-Malta version of the code has been used for the reproduction of the $^{58}Ni(n,x)$[4] and $^{A}Sn(n,x)$[5] (where A represents different isotopes of Sn) reaction cross-sections. There are four different level density models

[3]KALMAN code for generating and fitting experimental data developed by T. Kawano.
[4]see section 5.9.1
[5]see section 5.10

available in the EMPIRE-3.2.3-Malta code, which were used for the fitting of the experimental data. The pre-equilibrium models were also tested for the mentioned data in order to check the feasibility of the code to predict the PE contribution in the reaction data. The details regarding the level density and PE models are provided briefly in the following subsections.

4.2.1 Level density models in EMPIRE-3.2.3-Malta

There are four level density model included in the EMPIRE-3.2.3-Malta package, which can be selected by using the "*LEVDEN 0-3*" keyword in the input file of the code. The models stands for...

- LEVDEN 0: Fermi Gas Model [9], which is adjusted to the RIPL-3 database (default) database for the discrete levels
- LEVDEN 1: Generalised Superfluid Model [11, 12]
- LEVDEN 2: Gilbert Cameron level densities [35]
- LEVDEN 3: RIPL-3 microscopic HFB level densities.

Each of the level density model given above were tested to fit the cross-section data appropriately. The basic equation and the approach for the level density has already been discussed in section 4.1.1.

4.2.2 Pre-equilibrium models in EMPIRE-3.2.3-Malta

EMPIRE-3.2.3-Malta is equipped with the two phenomenological pre-equilibrium models, first is the Exciton model (PCROSS) [28] and second, the Monte Carlo Preequilibrium (DDHMS code) [29]. The exciton model is based on a master equation proposed by Cline [36] and Ribansky [37]. The equation consists of exciton number n and the decay probabilities of different neighboring states. The spin of decaying particles is not included in PCROSS formulation. However, it includes the probabilities of the cluster emission by using the improved version of Iwamoto Harada model [38]. On the other hand, the DDHMS code was developed by M. Blann [39] using the hybrid model [40–43] using intranuclear cascade approach. Since it uses Monte Carlo approach, thus, there is on limit for the pre-equilibrium emissions to take place. The DDHMS model has been tested and it performs well for most of the projectile target combinations up to 250 MeV incident energies. In addition to this, there are some constraints in order to use pre-equilibrium calculations together with different reaction models. The EMPIRE-3.2.3-Malta version has four modules for pre-equilibrium calculations, Multi-Step

Direct (MSD) [44], Multi-Step Compound (MSC) [27], HMS and PCROSS. The MSD and MSC calculations can not performed together with either HMS or PCROSS. But HMS and PCROSS can be combined as they excludes each other. In the present work the PE calculations were switched *'on'* and *'off'* by using the mean free path (*MFP*) parameter.

4.3 ALICE-2014 Nuclear Model Code

The Alice code has been used extensively for light and heavy-ion induced reaction data. It is based on the Monte Carlo (MC) precompound model [39]. The MC approach allows many body decay during the precompound phase and is limited only by the excitation energy. The incident particles can be taken from γ, n, p to any heavy-ion beam up to $\approx$ 200 MeV single particle energies. ALICE can be used for the calculation of reaction cross-section data, light excited nuclei may be given by the Fermi breakup option in decay [45], precompound+compound emission of ^{2}H, ^{3}H, ^{3}He, α, and ^{7}Be may be requested [46]. Isomer ratios can be calculated for product yields [47]. Targets having different isomers can also be assigned in the input description of the code. ALICE may be used for the calculations of the mass and charge fission yields long with their excitations [45]. The emitted n, p, α-particle spectra can also be obtained from a decaying nuclei. Double differential cross-sections (DDCS) [50] can be calculated or nucleon induced reactions by using the Chadwick and Oblozinsky model [48, 49]

4.3.1 Level density models in ALICE-2014

The particle level density parameter (PLD, a=A/k, where k is PLD parameter) can be adjusted by invoking the PLD input parameter in ALICE input. The PLD is set as 9 for default but it can be changed by the user according to reaction system. Other than this, there are four level density models included in the ALICE-2014 model which are...

- Fermi gas densities (default)
- Kataria and Ramamurthy
- Obninsk model
- Gilbert-Cameron model

In the present work, we have chosen the default input description for most of the cases under investigation. Obninsk level density model was also tested for the prediction of the proton-induced reaction cross-section data.

In summary, the TALYS-1.9 code has been used as the main tool for the theoretical calculations. In addition to TALYS-1.9, ALICE-2014 and EMPIRE-3.2.3-Malta were used for the comparison and validation of the theoretical codes itself. The purpose for the comparison was to check and validate the results of different codes using the similar input data. This would be helpful for other users to build confidence over EMPIRE and ALICE for the prediction of nucleon-induced reaction cross-section data.

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