Chapter 3

Theoretical Calculations

3.1   Introduction

In Chapter 1 and 2, the discussions revolves around the mechanism of neutron interaction and the overview of the experimental facilities utilized for the study of neutron induced reactions for reactor materials. The validation of the experimentally measured reaction cross section data are also important to gain the confidence to researchers for optimization of reaction phenomena. For validation studies, the reactions cross section were theoretically predicted by nuclear codes such as TALYS and EMPIRE. In cross section measurements various parameters will affect the results. Therefore, the nuclear codes are structured in such a way that for different interaction mechanism and reaction channels, the reaction cross section can be determined at different energies.

3.2   TALYS code

TALYS is a nuclear models based computer program to simulate the interaction mechanism for neutrons, photons, protons, deuterons, tritons, ^{3}He- and α-particles over a wide energy range from 1keV to 200 MeV [1]. The fundamentals of the interaction between the particles and nuclei can be analysed by interplaying the experimental and theory data which enable to construct physics model for precise measurements. By using this model, TALYS can generate the data to check the reliability in predicated data. After constructing the physics model, it will be used to generate the nuclear data for other reaction channels with fine-tuning the adjustable parameters. TALYS can generate the nuclear data for all reaction channels where no measurement are available for various energy and angle grid. Due to its precise and reliable data predication capability, TALYS code have many applications in fission-fusion reactors, transmutation of radioactive waste, accelerator technologies, medical isotope production, radiotherapy, oil-well logging, geophysics and astrophysics.

In TALYS code the input parameters are classified in various models for the level densities, direct reactions, compound reactions, pre-equilibrium reactions, fission reactions, optical

model and a large nuclear structural database, presented in *Figure 3.1*. The detailed description of these parameters are summarized in TALYS manual [1].
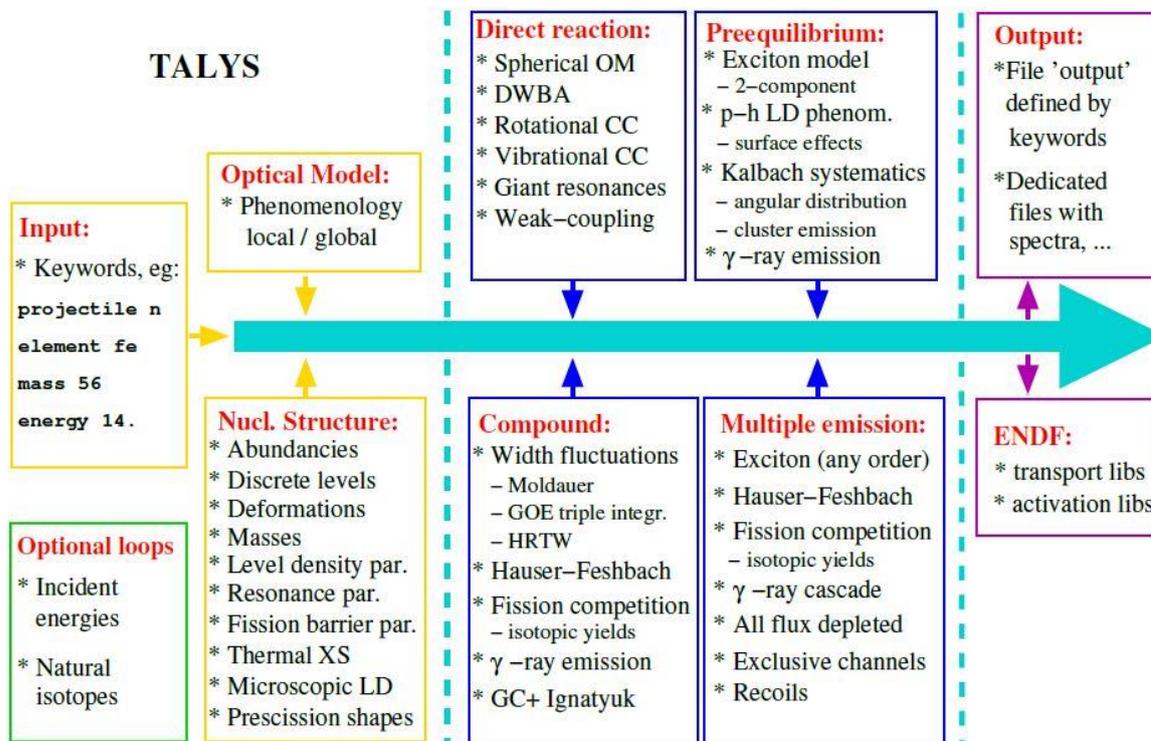

Figure 3.1 Nuclear model structure in TALYS code

In TALYS code, the basic input file structure to calculate the reaction cross section is as followed:

projectile n
element zr
mass 90
energy 16.99

In present work, the reactions cross section were predicted by considering the level density models and other fitting adjustable parameters such as optical model, densities of exciton model constituents, pre-equilibrium gamma emission, branching ratio etc. were taken as default.

Level Density Models (ldmodel) in TALYS

In TALYS, several models were used for the level density, which range from phenomenological analytical expressions to tabulated level densities derived from microscopic models. The complete details for phenomenological models can be found in Koning et al. [2].

ldmodel 1: Constant Temperature + Fermi gas model (CTM) [3]

ldmodel 2: Back-shifted Fermi gas Model (BFM) [4]

ldmodel 3: Generalised Superfluid Model (GSM) [5]

ldmodel 4: Skyrme-Hartree-Fock-Bogoluybov level densities from numerical tables [6]

ldmodel 5: Gogny-Hartree-Fock-Bogoluybov level densities from numerical tables [7]

ldmodel 6: Temperature-dependent Gogny-Hartree-Fock-Bogoluybov level densities from numerical tables [8]

Pre-equilibrium model in TALYS

The intermediate reaction having both direct and compound reactions like features referred as pre-equilibrium, precompound or in a quantum-mechanical context multi-step process. Pre-equilibrium processes includes the reaction cross section for incident energies between 10 to 200 MeV. For enabling the pre-equilibrium model, term 'preeqmode' used in the input file which have four possibilities where 'preeqmode 2' is the default model [9-11]. The Pre-equilibrium process of the excited nucleus is presented in *Figure 3.2*. In TALYS two versions of the exciton model are implanted. The default is the two component model and there are four possible pre-equilibrium models are available in input as follow:

preeqmode 1: Exciton model: Analytical transition rates with energy-dependent matrix element.

preeqmode 2: Exciton model: Numerical transition rates with energy-dependent matrix element.

preeqmode 3: Exciton model: Numerical transition rates with optical model for collision probability.

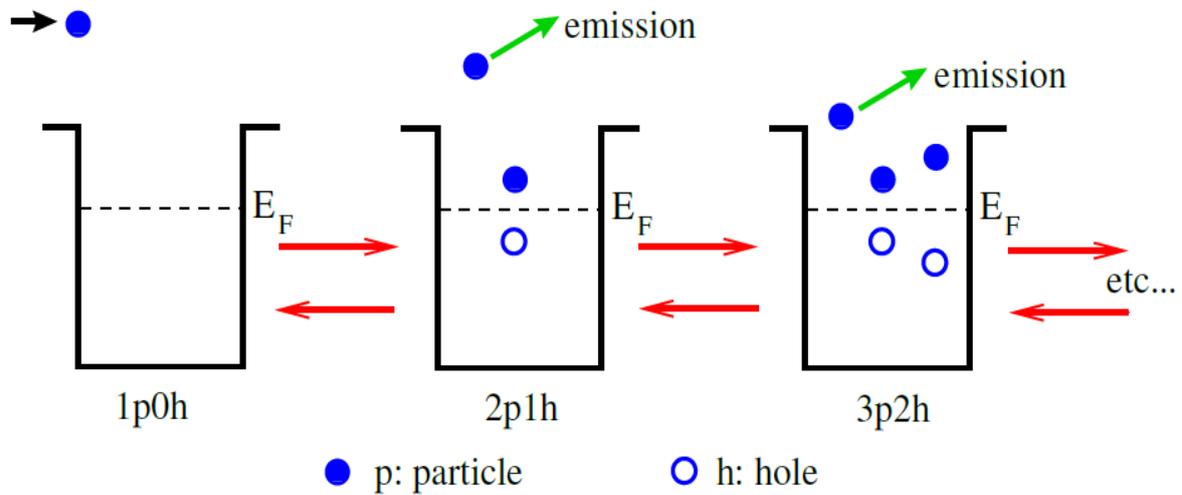**preeqmode 4:** Multi-step direct/compound model

Figure 3.2 Reaction flow in exciton model

3.3   EMPIRE code

EMPIRE code is served as a tool for modeling the nuclear reactions through the application of different theoretical models over a wide energy spectrum. The interaction mechanism is models by selecting neutron, proton, deuterons, tritons, helions (^{3}He), α-particles and light or heavy ions as projectile. The energy range for neutron induced reactions starts above the resonance region and for heavy ion induced reactions extends up to few hundred MeV [12]. EMPIRE code comprises of direct reactions which are referred by a generalized optical model (ECIS06 or OPTMAN) or simplified coupled-channels approach. The pre-equilibrium reactions are taken care by deformation dependent multi-step direct (ORION + TRISTAN) model or by exciton model (PCROSS) [13]. The compound reactions are described by Hauser-Feshbach model with γ-cascade and width fluctuation [14-16]. The basic nuclear model structure used in EMPIRE code is presented in *Figure 3.3*.
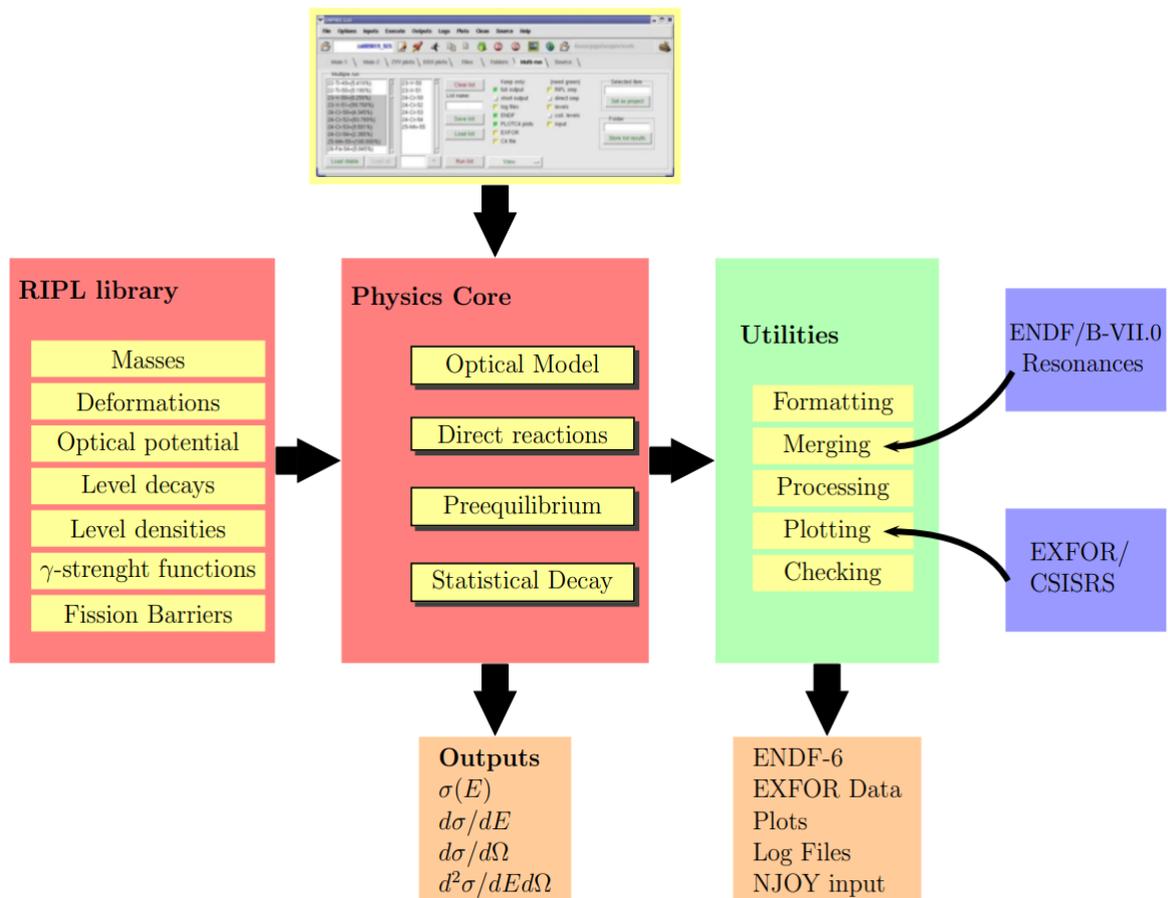
Figure 3.3 Nuclear model structure in EMPIRE code

The input file structure for EMPIRE code is as followed:

16.99   ; INCIDEN ENERGY (IN LAB)

90. 40.   ; TARGET A, Z

 1.   0.   ; PROJECTILE A, Z

2   ; NUMBER OF NEUTRONS TO BE EMITTED

1   ; NUMBER OF PROTONS TO BE EMITTED

1   ; NUMBER OF ALPHAS TO BE EMITTED

1   ; NUMBER OF DEUTERONS TO BE EMITTED

0   ; NUMBER OF TRITONS TO BE EMITTED

0   ; NUMBER OF He-3 TO BE EMITTED

0   0.   .   ; reserved

Besides this input parameters, several fitting parameters are available to predict the best fit reaction cross section.

Level Density Models (LEVDEN) in EMPIRE

In EMPIRE different level density formulations are provided with different parameters defined as 'LEVDEN' in input file. There are four possibilities are available for LEVDEN model specified as,

> **LEVDEN 0:** EMPIRE specific level densities, adjusted to RIPL-3 experimental D_{obs} and to discrete levels (default) [3],
>
> **LEVDEN 1:** Generalized Superfluid Model (GSM) adjusted to RIPL experimental D_{obs} and to discrete levels [5, 6],
>
> **LEVDEN 2:** Gilbert-Cameron level densities adjusted to RIPL experimental D_{obs} and to discrete levels [17],
>
> **LEVDEN 3:** RIPL-3 microscopic HFB level densities.

Pre-equilibrium model in EMPIRE

In EMPIRE two pre-equilibrium models are available for the cross section calculations. The classical exciton model (PCROSS) is the first model which includes nucleon [13], cluster and gamma emissions. The second is the Monte Carlo DDHMS inspired by Blann's Hybrid model limited to nucleon emission [18-22]. The former includes only the first pre-equilibrium emitted particle and is therefore valid up to about 50 MeV. The latter also includes multiple pre-equilibrium emission, which extends its applicability to much higher energies. The exciton model code DEGAS implementing full angular momentum coupling in pre-equilibrium emission of nucleons and gammas has been temporarily disabled due to incompatibilities with the current system.

PCROSS

The module PCROSS includes the pre-equilibrium mechanism as defined in the exciton model [12].

> **PCROSS = 0,** PCROSS disabled (default)

PCROSS > 0, PCROSS enables with mean free path multiplier set to value. The value must be greater than 0.5 and lower than 3.

HRTW

Hofmann, Richert, Tepel and Weidenmueller (HRTW) proposed a model for the correlation between the incident and exit channels in elastic scattering used in EMPIRE code. This model is used for the width fluctuation correction in computation.

HRTW = 0, Disabled HRTW

HRTW > 0, HRTW width fluctuation correction applied up to the defined energy value.

GSTRFN

EMPIRE code includes six γ-ray strength functions, defined as 'GSTRFN'. This function controls the modeling of the γ-ray strength function.

GSTRFN = 0 enhanced Generalized Lorentzian EGLO (Uhl-Kopecki) [23]

GSTRFN = 1 modified Lorentzian version 1 MLO1 [24]

GSTRFN = 2 modified Lorentzian version 1 MLO1 [25]

GSTRFN = 3 modified Lorentzian version 1 MLO1 [26]

GSTRFN = 4 enhanced Generalized Lorentzian [11]

GSTRFN = 5 GFL (Mughabghab) [27]

GSTRFN = 6 SLO standard Lorentzian [28]

OMPOT

The 'OMPOT' keyword selects optical model parameters for the outgoing particle. The input file can be defined as 'OMPOT VALUE I1' in which VAL must be set to a RIPL catalog number (e.g. 2408 for Capote et al OMP) of the potential as it appears in the empire/RIPL/optical/om-data/om-index.txt file or in Help=> 'RIPL omp" for GUI. For backward compatibility this number can be entered with a negative sign.

OMPOT = 1 for neutrons,

OMPOT = 2 for protons,

OMPOT = 3 for alphas,

OMPOT = 4 for deuterons,

OMPOT = 5 for tritons,

OMPOT = 6 for 3He.

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