Chapter 3

THEORETICAL ASPECTS

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3.1 Introduction

Theoretical aspects related to present work are covered in this chapter along with the experimental and theoretical reaction cross-section data available in the IAEA sites [1, 2]. Detailed discussions of Nuclear Model codes TALYS [3, 4] and EMPIRE [4, 5] as well as EXFOR [1] and ENDF [2] are described in this chapter. Nuclear model code discussion is followed by the brief discussion of data libraries, which are available online, including theoretical calculations as well as measured experimental data. When there is a scarcity of experimental data in the literature, theoretical data can provide the useful insight of reactions of interest. Hence, there is a need of theoretical as well as experimental data. Theoretical nuclear model computations are of extreme importance for the advanced nuclear data analysis methodology. In last few years profound improvement can be reached in the capabilities of theoretical models for predicting the neutron induced reaction cross-sections in the range where there is a scarcity of experimental data. These calculations are useful to interpolate and extrapolate neutron cross-section data, to minimize the discrepancies between different experimental data and for some materials, in some energy regions where there is no measured data available, mainly in MeV region [6]. Several computer codes employing various nuclear reaction mechanisms were developed for the calculation of cross-section, particle spectra, fission yields, angular distribution etc. The codes are of different in terms of complexity. These codes use different approaches and have ranges of different applicability [7, 8].

3.2 TALYS

TALYS is a nuclear reaction simulation code that includes nuclear reactions considering neutrons, gamma-rays, protons, deuterons, tritons, and alpha-particles as a projectile, with the energy range of 1 keV to 200 MeV [3]. Different nuclear reaction models have been combined into a single code system, which enables us to analyse nuclear reactions beyond the resonance region. Main nuclear models, such as currently advanced optical models, compound nucleus, fission, level density, gamma-ray strength and pre-equilibrium models, all these are govern by a encyclopaedic database. The validity and reliability of the code is manifested by the comparison of the computed results with a distinct set of measured data from 1 keV to 200 MeV. Thus, TALYS is a powerful outlook that covers the whole path from fundamental nuclear reaction models to the creation of complete data libraries for nuclear applications.

3.2.1 Overview

The computer code TALYS is a nuclear model code developed by A. J. Koning in the year 2003. Simulation of Nuclear reactions can be done using this code. It is a Linux operating system based code and it needs FORTRAN or C language as a compiler. TALYS-1.0 is the very first version of TALYS code and was out in 2007. After that it was further modified, i.e., TALYS- 1.2, 1.4, 1.6, 1.8. TALYS 1.8 is the advanced version available in the market these days. In light particle induced reactions, to cover almost all chief reaction mechanisms, several nuclear models were included in the code. It is a code that provides a complete description of all the reaction channels. It is a reliable tool to generate nuclear data. This computer code can be used to calculate the reaction cross-section based on physics models and parameterizations. It calculates nuclear reactions involving targets with mass larger than 12 amu and projectiles like photon, neutron, proton, ^{2}H, ^{3}H, ^{3}He and alpha particles in the energy range from 1 keV to 200 MeV. One can calculate partial and total cross-sections, energy spectra, angular distributions, double differential spectra and recoils, discrete and continuum photon production cross-section, excitation functions for reaction products and isomeric cross-sections. The official web site is http://www.talys.eu/home. This code uses a reference input parameter library (RIPL). Automatic reference to nuclear structure parameters as masses, discrete levels, resonances, level density parameters, deformation parameters, fission barrier and gamma-ray strength function mainly from IAEA RIPL is used. In RIPL different level density models, various fission models for the prediction of fission fragments and product yields, models for pre-equilibrium reactions up to any order astrophysical reaction rates using Maxwellian averaging are included. There are options for the user to start with the excitation energy distribution instead of just projectile-target combination. One can use systematics if for a particular reaction mechanism is yet not available and thus can use this code as an alternative predictive model [3].

3.2.2 RIPL (Reference Input Parameter Library)

Appropriate input file and parameter library are mandatory for the development of advanced codes. So the International Atomic Energy Agency (IAEA) developed a library, which contains validated nuclear-model input parameters, referred to the Reference Input Parameter Library (RIPL) [4]. It took fifteen years for IAEA to build final RIPL coordinated research project (RIPL-3) since 1993 to 2008. The RIPL-3 library was made available through http://www.nds.iaea.org/RIPL-3/ on January 2009 (Capote et al., 2009). The RIPL

and the final database are of great importance for theoreticians who are associated with the development and use of nuclear reaction modelling (ALICE, EMPIRE, GNASH, TALYS) [4].

3.2.3 Different nuclear models related to TALYS

1. Optical model
2. Direct reactions
3. Compound reactions
4. Level densities
5. Pre-equilibrium reactions
6. Multiple emissions
7. Fission
8. Nuclear structure database

3.2.4 Different level densities

1. Gilbert-Cameron model
2. Back shifted Fermi gas model
3. Super fluid model
4. Ignatyuk damping of shell effects in the level density parameter
5. Rotational/Vibrational effects
6. Microscopic level densities, based on Hartree-Fock-Bogolyubov model, parity-dependent nuclear level density

3.2.5 How to run TALYS code

TALYS input file containing keywords and their appropriate values is a necessity for running TALYS successfully. There are four main keywords: projectile, element, mass and energy.

Projectile: Projectiles can be selected from n, p, d, t, α,.. In our case neutron is a projectile.
Element: One can choose periodic table's any of the elements as a target. In the present work Au, Mn, Th and U are taken as target.
Mass: The element mass must be written in front of the keyword mass. For the present work, mass of Au is 197, mass of Mn is 55, and masses of Th and U are 232 and 238, respectively.

Energy: The energy keyword asks for the incident energy of projectile, which causes nuclear reaction and to be measured. This key word may contain a single value of energy as well as a range of different energies. If one wants to choose range of different energies, it should be given another name instead of a number. An energy file having the same name must be present in the sample model, whichever we want to run. This file name is case sensitive. To understand it easily, we have given the example of TALYS input file for the calculation of neutron induced reaction cross-sections of ^{197}Au below:

projectile n
element Au
mass 197
energy energies

"energies" file containing different energies is names as energies, and will be the same as one given below:

1
2
.
.
.
.
20

All these energies written in energy file are considered to be in MeV range.

The command to run this input file along with this energy file is as follows:
talys< input > output

After running this TALYS input file, one will get the output file containing different segment. Each segment has a different significance based on the values fed against these key words.

3.2.6 Output quantities calculated with the help TALYS

Cross-sections:

1. Total cross-sections
2. Shape-elastic cross-sections

3. Compound elastic cross-sections
4. Inelastic cross-sections
5. Nuclear reaction cross-sections
6. Inelastic cross-sections, per level and total
7. Residual production cross-sections
8. Total particle production cross-section
9. All exclusive reaction channels (e.g., (n,n'), (n,dt),...)
10. All exclusive isomer production cross-sections
11. All exclusive discrete and continuum γ-ray production cross-section.

Spectra:

1. Elastic angular distributions
2. Inelastic angular distributions and energy spectra
3. Tabulated angular distributions or Legendre coefficients
4. All exclusive double-differential spectra
5. Total particle production spectra
6. Compound spectra per reaction stage
7. Multi-pre-equilibrium spectra per reaction stage

   We have kept our output limited to total cross-section values and level densities were set as default.

3.3 EMPIRE

EMPIRE is also a model based code for nuclear reaction computations [5]. It can evaluate the cross-section data with the use of projectiles like neutrons, gamma-rays, protons, deuterons, tritons, hellions, alpha-particles, light or heavy ions. The range of these incident projectiles is from few keV to few hundred MeV. It enables us to generate almost all the nuclear reactions beyond the resonance range. EMPIRE represents a user friendly computational approach which holds the full data libraries having nuclear applications [5].

3.3.1 Overview

Dr. Michale Herman, BNL (USA) developed the nuclear reaction code EMPIRE in 2007 [5]. It is a combination of several model codes. In fact, EMPIRE is a combination of the original coding of Herman and several codes written by other authors. This system is based on a specific nuclear reaction model and used for nuclear reaction calculations. EMPIRE is a

Linux based program and also there is a window version available. This model code is designed in such a way that it can calculate cross-sections over a large range of energies and incident particles. It is a user friendly code. One can use a light ion (proton, deuteron, or alpha particle), uncharged particle (neutron or photon) or heavy ions as a projectile. The energy range starts from the unresolved resonance region for neutron induced reactions (~ keV) and continues up to several hundred MeV for heavy ion induced reactions. EMPIRE 3.0 has achieved practically almost all the goals that were set up in the conceptual design of the code so one can count this version of a code as a milestone in the evolution of this code. This nuclear model code is a theoretical tool for basic research and nuclear data evaluation for calculation of nuclear reaction cross-sections in a wide range of incident projectiles possessing different energies. Similar to TALYS, RIPL (Input parameter library) is used along with CCFUL in EMPIRE [4].

3.3.2 Different nuclear reactions

- Direct reactions
- Pre equilibrium emission
- Compound Nuclear reactions

3.3.3 Different reaction models associated with EMPIRE

1. Optical model
2. DWBA (Distorted Wave Born Approximation)
3. Couple Channels
4. MSD (Multi-step Direct)
5. MSC (Multi-step Compound)
6. Exciton Model (PCROSS) Hybrid Monte Carlo Simulation
7. Full Featured Hauser-Feschbach model

3.3.4 Description of the code

a) The input parameters to the code:

The nuclear structure inputs like

b) Flow of calculations

1. Read input file (*.inp)
2. Construct table of nuclides involved

3. Read from RIPL data:

a) Discrete levels

b) Binding energies

c) Level density parameters

d) Shell corrections

e) Ground state deformations

f) Optical model parameters

4. Calculate

a) Transmission coefficients

b) Level densities

5. Retrieve experimental data from EXFOR library

6. Write input/output files (*.lev, *-omp.int, *.exfetc)

7. Determine fusion cross-section

8. Select the compound nucleus for consideration

9. Calculate n, p & γ emission spectra in terms of exciton model (DEGAS)

10. Calculate n, p & γ emission spectra (MSC mechanism)

11. Calculate n, p, α & γ emission spectra in terms of exciton model (PCROSS)

12. Calculate n, p, α & γ emission widths in terms of Hauser Feshbach statistical model.

13. Print result for decay of nucleus considered

14. Select new nucleus and repeat H-F calculation until all nuclei are processed

15. Read new incident energy (from input file) and repeat step 4 and 7 onwards till all requested energies are done.

3.3.5 How empire executes

Execution of the code EMPIRE is done step by step, which is explained in following steps:

1. First of all, one has to specify the project NAME, i.e., Au197.
2. After that one has to generate an input file, i.e., Au197 with the help of CREATE command.
3. Only the input file Au197 should be kept and everything else should be removed with the help of ROOT Au197.
4. Input file should be executed with the necessary parameters from the RIPL library, with the help of RUN command.

5. EMP-FULL and EMP-SHORT indicates the input files having full and brief description, respectively.
6. To modify files as per the needs OMP is used.

3.3.6 Input parameters

Nuclear masses, discrete energy levels and level densities of the nuclides, all these nuclear structure input parameters are taken from the latest compilation available in RIPL-3 [4]. Other input parameters are manually fed in the input file.

The input to the code comprises of two parts.

a) Necessary input

0.1 : incident energy (in lab)
232 90 : target A, Z
1 0 : projectile A, Z
1 : number of neutrons to be emitted
0 : number of protons to be emitted
0 : number of alphas to be emitted
0 : number of deuterons to be emitted
0 : number of tritons to be emitted
0. 0. 0. : number of L.I to be emitted and it's A and Z

The first line gives the information of the incident energy (MeV) in the laboratory system. Second and the third lines are used to specify the masses and atomic numbers of a target and a projectile respectively. The next five lines define the number of emissions to be followed for each ejectile. The last line of the input provides for the inclusion of the emission of one type of light ion. The library of optical model parameters allows for d, t, ^{3}He, ^{6}Li, ^{7}Li and ^{7}Be ejectiles.

b) Optional input

The mandatory input is followed by the optional input which allows modifications to the default model parameters. Optional input consists of an arbitrary number of records entered in any order and closed with GO record. Each record starts with an alphanumeric keyword NAME, which is followed by the value VAL and the positional parameters.

Keyword indicates a physical quantity like the binding energy or level density parameter or an option. VAL takes the numerical value of the quantity or option and positional parameters are used to specify to which nucleus the quantity should be applied.

The optional input with default value of parameters

Keyword Description Default value

NEX Controls maximum number of Energy

Steps in the integration

50

ENDF Controls output for ENDF formatting 0 (NO)

IOUT Controls the main output 1

HRTW Controls width fluctuation calculations 1

DIRECT Controls coupled channel calculations 0

MSD Controls multistep direct calculations 0 (NO)

MSC Controls multistep compound calculations 0 (NO)

DEGAS Controls Exciton model calculations 0 (NO)

HMS Monte-Carlo Pre-equilibrium calculations 0 (NO)

PCROSS Exciton model with cluster emission 0 (NO)

LEVDEN Selection of level density approach 3 (HFB)

=0 Default level densities will be selected from RIPL-3 adjusted to discrete levels

=1 GSM (Generalised Superfluid Model) adjusted to discrete levels

=2 GC (Gilbert-Cameron level densities) adjusted to discrete levels

=3 Microscopic HFB (Hartree-Fock-Bogolyubov) level densities, Parity dependent

=4 Gilbert and Cameron level densities

ATILNO Escalation parameter set to value VAL

OMPOT

Optical model potential selection from

RIPL-3

-2405 (n) (Koning)

-5405 (p) (Koning)

-9600 (α) (Avrigeanu)

-6001 (d) (Perey)

DIRPOT direct reaction contribution

3.4 Data libraries

Nuclear data available in the literature can be classified in three main categories:

1. Measured/ Experimental nuclear reaction data (EXFOR)
2. Computed/Theoretical nuclear reaction data (ENDF)
3. Nuclear Structure and decay data along with the nuclear levels, half lives and radioactive decay radiations

3.4.1 EXFOR

EXFOR stands for Exchange FORmat, which is data library with format for the collection, storage, exchange and retrieval of experimental data [1]. EXFOR is an international data library co-operated by NRDC (Network of Nuclear Reaction Data Centre) co-ordinated by the International Atomic Energy Agency (IAEA). The web site for the same is www-inds.iaea.org. It has a mirror site operated by NDS (Nuclear Data Section). The mirror web site is www.nndc.bnl.gov.

3.4.2 ENDF

ENDF stands for Evaluated Nuclear Data Format [2]. This data library contains the evaluated data. These data are achieved by the analyses of the available experimentally, measured data and combination of both of them with the nuclear model code calculation. There are different evaluated data libraries under ENDF and they are as follows:

ENDF (USA) [2]
JEFF (Europe) [9]
JENDL (Japan) [10]
CENDL (China) [11]
ROSFOND (Russia) [12]
BROND (Russia) [13]

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