Chapter 6

Study of deuteron induced reactions using statistical model codes

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The examination of the effect of nuclear reaction is important to study, which is used as a building material in nuclear reactors. Nuclear reactions occur as a outcome of projectile and target interaction. The charged particle-induced reactions have prime importance to gain the knowledge about reaction mechanism which can be applied to understanding the particles resulting from the reaction. It is useful to develop the shielding of the particle accelerators and fusion reactors. The present study contributes in providing the theoretical prediction of excitation functions for ^{112}Cd(d, 3n)^{111}In, ^{141}Pr(d, 3n)^{140}Nd, ^{167}Er(d, 3n)^{166}Tm, ^{197}Au(d, 3n)^{196}Hg, and ^{209}Bi(d, 3n)^{208}Po reactions using theoretical model codes such as TALYS (v. 1.95), EMPIRE (v. 3.2.3), and ALICE-2014 from threshold energy to 50 MeV of deuteron energy. Also, the calculation was performed utilizing newly developed (d, 3n) formula of Y. Kavun (2020) for these reactions at 20 MeV of deuteron energy. Lastly, all calculated results were simulated with one another and with the previously published data of the EXFOR data library.

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6.1 Introduction

Awareness of the cross section of deuteron-nucleus interaction is essential for both fundamental and application based nuclear research [1]. In recent years, the nuclear data of deuteron induced reactions have captivated much interest in the variety of field related to neutron applications as they can produce high-intensity neutrons [2]. The deuteron induced reactions have various applications which are mentioned below [3].

- Space applications such as shielding, the resistance of electronics, etc.;
- Accelerators produces high intensity, high energy neutron fluxes for nuclear waste transmutation in ADSs [3];
- Intense neutron sources (EVADA/IFMIF, SNS, ESS, ARC neutron activators) [4];
- Production of the radioactive ion beam (RIB) with neutrons (SPIRAL-2, EURISOL, RIA, etc.) [5];
- Future controlled fusion reactors and experiments (DEMO, ITER, etc.);

Further, a systematic study is scarce for reactions produced by deuteron in contrary to proton and alpha-nucleus interaction [1]. Indeed, the mechanism of these reactions is more complex than the other charged particle reactions as the deuteron is a loosely bound nucleus.

The deuteron has very low binding energy, $B_d = 2.225$ MeV, and can easily break up in the Coulomb and nuclear fields of a target nuclide. Therefore, the complex interaction takes place which includes a variety of proton and neutron reactions started from the breakup of deuteron. This wide diversity of reactions hampering the detailed analysis including a wide range of target samples and domain of incident energy [6, 7]. Also, We are aware that the evaluated and experimental data related to the deuteron reaction are less accurate and extensive than the data of neutrons. Therefore, improved model calculation and more measurements are required [8]. The ongoing project of FENDL-library [9] has also motivated for the deuteron data and complexity of deuteron interactions.

Therefore, a systematic study was on certain metals of the Periodic Table such as ^{112}Cd, ^{141}Pr, ^{167}Er, ^{197}Au, and ^{209}Bi in the present work. The chosen elements are essential in variety of fields like nuclear technology and physics as well as in nuclear medicines. The chosen element ^{112}Cd is used for investigating wear control utilizing thin layer activation (TLA) method, in the yield production of long lived isotopes required for waste handling and dose estimations [10], for the medical based isotopes production [11]. Further, the deuteron induced (d, 3n) reaction on the mono-isotopic element ^{141}Pr produces ^{140}Nd as a product nucleus which is expected to use in Positron Emission Tomography (PET) [12]. Erbium is a rare-earth metal, used as a control rod for the neutron absorber in nuclear technology. It can also used for thulium and erbium radionuclides production which are important in medical sectors [13, 14]. Gold is a monotonic element, and theoretical calculations are easier to compare [1]. Gold is also utilized as a flux monitor reaction for the neutron flux estimation. Bismuth is used for the radiation shielding nowadays and also an excellent material for ADSs [15].

The excitation functions of (d,3n) reaction have been studied from the threshold energy to 50 MeV of deuteron energy for the chosen isotopes using the newest version of statistical model codes TALYS [16], EMPIRE [17], and ALICE [18]. The (d, 3n) empirical formula systematic developed by Kavun (2020) [19] has been also used to calculate the excitation function for the energy 20 $\pm$ 1.5 MeV. The resultant values are compared with the dataset of TALYS, EMPIRE, and ALICE, also with the EXFOR data library [20].

6.2 Calculation methods

6.2.1 Cross-section formula systematic

Many studies can be found in the literature related to empirical formula systematics for the cross section determination [21–25]. It is observed from the previous studies that the cross sections of the target nucleus depend on mass number (A), neutron (N), and proton (P) numbers. Levkovskii has defined asymmetry parameter as (s = (N - P)/A) [25], by considering the dependence effects of the isotonic, isotopic, and odd-even properties of nuclei variables.

The proposed Levkovskii formula for reaction systematic is [25]:

$$\sigma(n, x) = C\sigma_{ne}e^{\alpha(N-P)A} \tag{6.1}$$

Here, σ_{ne} represents the nonelastic cross-section parameter. Also, C & α are obtained from the least square fitting. A similar systematic is used for (d, 3n) reactions by [19]. The obtained cross section formula for the mass range $45 \leq A \leq 112$ & $124 \leq A \leq 239$ at 20 ± 1.5 MeV has been given in Table 6.1.

Table 6.1: The empirical formula for (d, 3n) reactions at 20 ± 1.5 MeV [19].

Mass region	B	a	$\sigma(d, 3n) = B(A^{1/3} + 2^{1/3})^2 \exp(as)$	R^2
$45 \leq A \leq 112$	0.003274	56.738	$\sigma(d, 3n) = 0.003274(A^{1/3} + 2^{1/3})^2 \exp(56.738s)$	0.863
$45 \leq A \leq 209$ (Even N - Odd Z)	0.04391	32.496	$\sigma(d, 3n) = 0.04391(A^{1/3} + 2^{1/3})^2 \exp(32.496s)$	0.815

6.2.2 Theoretical model calculation

Theoretical calculations were performed for the simulation purpose of the present study. The latest versions of TALYS [16], EMPIRE [17], and ALICE [18] have been adopted for the same. A detail description of these codes is given in Chapter 3. The different nuclear models have been prepared to cover all main reaction mechanisms in these codes. TALYS contains six NLD models, EMPIRE consists of four NLD models and ALICE contains four NLD models. The calculation was performed using the default NLD option of all three codes from threshold energy to 50 MeV of deuteron energy for every reaction.

6.3 Result & Discussion

Two commonly utilized parameters to identify the various radiation interaction of building materials in nuclear reactors caused due to radiation exposure are (i) neutron and charged particle flux, and (ii) Displacement per atom (DPA). The neutron flux in the medium relies on the characteristics of the irradiation source, whereas the detected flux for a source relies on the point where the flux is estimated, and on the interacting material [26]. It is assumed that low energy neutrons do not taking part to the material damage of the reactor. Therefore, it is considered that the neutron flux with an energy greater than MeV would cause damage to the building materials of the reactor. Initially, the limit was considered 1 MeV as a reference and then gradually it is adopted for many applications with neutron flux $>$ 0.1 MeV, and even older reactors in the USSR often used fluxes greater than 0.5 MeV [26]. Therefore, it is essential to investigate the characteristic of the elements of the periodic table such as ^{112}Cd, ^{141}Pr, ^{167}Er, ^{197}Au, and ^{209}Bi which are utilized for the construction of nuclear reactors for various purposes flux monitor, shielding, neutron flux control, etc. Although a good amount of study has been done on various materials for neutron induced reactions, some other reactions are crucial to study for the contribution of nuclear transmutation and damage study.

In the above context, we have considered the materials mentioned above and studied their interaction with the deuteron. We made the comparison of theoretical predictions of TALYS, EMPIRE, and ALICE with the EXFOR dataset and the cross section was computed utilizing the (d, 3n) systematic formula of Kavun (2020) [19] for ^{112}Cd(d, 3n), ^{141}Pr(d, 3n), ^{167}Er(d, 3n), ^{197}Au(d, 3n), & ^{209}Bi(d, 3n) reactions and plotted in the following figures, respectively. The default models of theoretical model codes are considered for the present study.

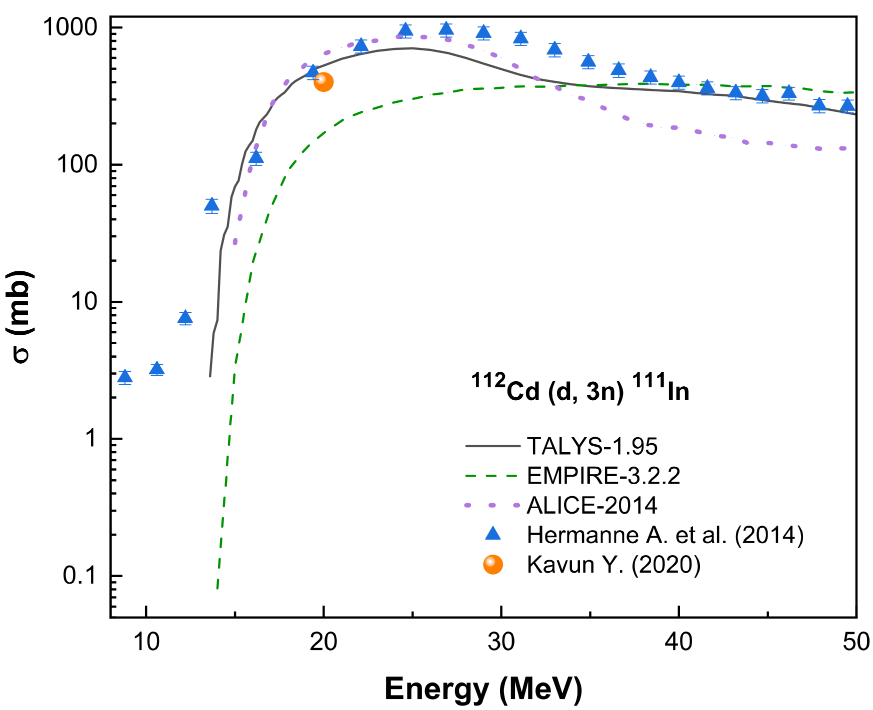

Figure 6.1: Comparison of theoretical predictions with EXFOR data, and the result of Kavun's empirical formula [19] for ^{112}Cd(d, 3n)^{111}In reaction.

The experimental data of $^{112}Cd(d, 3n)^{111}In$ reaction are retrieved from the EXFOR data library and simulated with the theoretical calculations of TALYS, EMPIRE, and ALICE codes as well as with the presently calculated value by systematic formula and plotted in Fig. 6.1. The outcomes of TALYS and EMPIRE start from nearly 14 MeV with 2.86 mb and 0.24 mb cross section values respectively. These data values increase up to around 20 MeV. The data of Hermanne *et al.* (2014) [27] are available from around 9 MeV to 50 MeV, which shows better agreement with the data predicted with TALYS above 13 MeV. However, the theoretical prediction of EMPIRE shows lower values till 35 MeV of deuteron energy. In addition to these results, the cross section value at 20 MeV was calculated using the empirical formula (Kavun, 2020), which gives the value of 400.95 mb. This result is agreed with EXFOR data, and also with the theoretical prediction of TALYS and ALICE and shows consistency with the theoretical predictions.

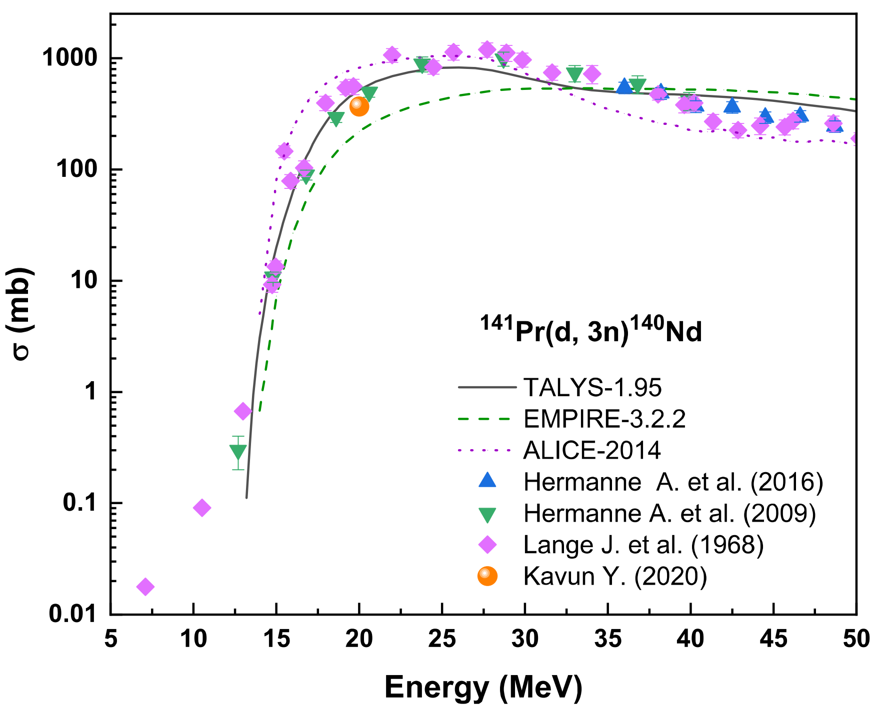

Figure 6.2: Comparison of theoretical predictions with EXFOR data, and the result of Kavun's empirical formula [19] for $^{141}Pr(d, 3n)^{140}Nd$ reaction.

Fig. 6.2 represents the analogy of theoretical data with the experimental data for the $^{141}Pr(d, 3n)^{140}Nd$ reaction having 13.018 MeV of threshold energy. The data extracted from the EXFOR data library follows the trend of theoretically predicted data. The previously reported measurements of Hermanne *et al.* (2016) [28] and Hermanne *et al.* (2009) [29] are analogous with data of TALYS, whereas the data of Lange and Müenzel (1968) [30] literature are slightly higher than TALYS data. However, the experimental data shows good agreement with ALICE data. EMPIRE predicts data lower than the other predictions and EXFOR data till 35 MeV of deuteron energy. The results of TALYS start from 13.2 MeV energy with a value of 0.111 mb and it increased till 27 MeV with 811.8 mb. After this deuteron energy, the values slightly reduced and at 50 MeV the value is 331.8 mb. EMPIRE calculation shows that the cross section value of 0.681 mb is obtained at 14 MeV, and the values increased up to 33 MeV. After the value of 535.8 mb at 33 MeV, these values gradually decreased. The cross section value was computed using the (Kavun, 2020) empirical formula is 367.97 mb at 20 MeV of deuteron energy and is well matched with TALYS data and with the EXFOR data.

For the calculation of Cd, and Pr, it is observed that the predicted data matches well with the EXFOR data available up to 50 MeV. Therefore, we can use a similar method to predict data for and ^{167}Er, ^{197}Au, ^{209}Bi. For these isotopes, the data set is not completely up to 50 MeV. The predictions agree with the available EXFOR data and further evaluation of data made up to 50 MeV using theoretical model codes TALYS, EMPIRE and ALICE. The new data set has been provided for higher energies where there is no experimental data available.

Figure 6.3 represents tan analogy between experimental data, theoretical data, and the calculated value with the systematic formula for the $^{167}Er(d, 3n)^{166}Tm$ reaction. The threshold energy of the reaction is 12.632 MeV of deuteron energy. The experimental data of Hermanne *et al.* (2011) are well matched with ALICE data as well as with data of TALYS. It is observed that the theoretical prediction of EMPIRE is higher than the predictions of TALYS after 26 MeV of energy and ALICE data are lower than the TALYS data after 27 MeV of energy. The cross section at 20 MeV calculated using the (d, 3n) (Kavun, 2020) formula is 567.6 mb and it is analogous with TALYS data.

It is noticeable from TALYS predictions that the value of cross section is 0.999 mb at 12.8 MeV of energy which increases gradually up to 21 MeV. After that the values of cross sections decrease at an almost constant rate and the final value is 108.4 mb at 50 MeV.

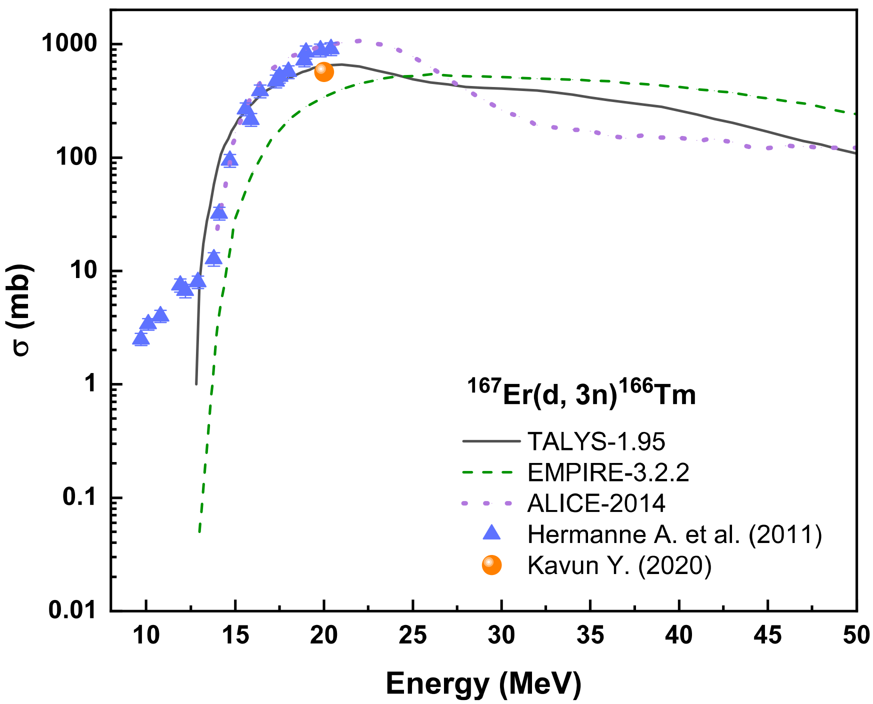

Figure 6.3: Comparison of theoretical predictions with EXFOR data, and the result of Kavun's empirical formula [19] for ^{167}Er(d, 3n)^{166}Tm reaction.

The cross section value of EMPIRE is 0.05 mb at 13 MeV of deuteron energy which increased up to 502.3 mb at 17.5 MeV. Then, the value decreases and it is 241.2 mb at 50 MeV of energy. The previously published data of Hermanne *et al.* (2011) [31] starts from 2.5 mb at 9.7 MeV and took the value of 268.6 mb at 15.6 MeV, which is compatible with the theoretically obtained data.

For ^{197}Au(d, 3n)^{196}Hg reaction, the comparison of the EXFOR data with theoretical calculation is plotted in Fig. 6.4. The TALYS data starts from 10.06 MeV deuteron energy with cross section value 0.0052 mb and it increased till 23 MeV with 721.9 mb. Then, the cross section value decreases to 157.7 mb at 50 MeV energy. While for EMPIRE, the results are started at 11 MeV and took the value of 0.016 mb. The cross section value increases up to 25 MeV of deuteron energy and then gradually decreases up to 50 MeV of energy with 212.5 mb of the cross section. The cross section value found at 20 MeV of deuteron energy is

1368.8 mb using the (d, 3n) empirical formula of (Kavun, 2020). The measured data point is in good agreement with ALICE data. These theoretical calculations were compared with EXFOR experimental data of Chevarier *et al.* (1970) [32] achieved 22 ± 7 mb at 10.8 MeV and 757 ± 189 mb at 20 MeV, then continued to decrease to 26 MeV, where it took the value of 380 ± 95 mb.

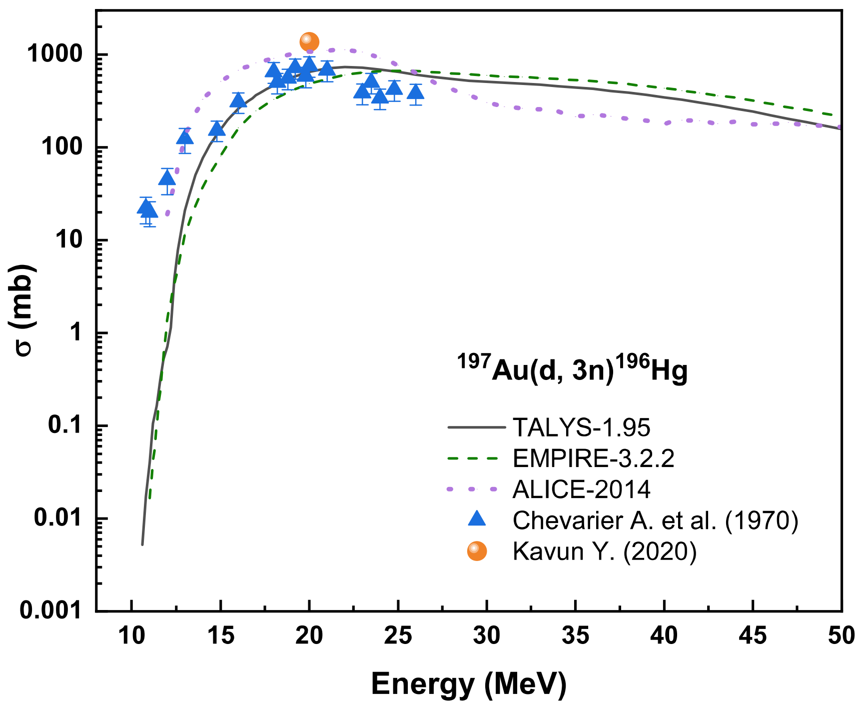

Figure 6.4: Comparison of theoretical predictions with EXFOR data, and the result of Kavun's empirical formula [19] for ^{197}Au(d, 3n)^{196}Hg reaction.

The ^{209}Bi(d, 3n)^{208}Po reaction having 11.986 MeV of threshold energy. The cross section comparison of previously published experimental data with theoretical predictions is presented in Fig. 6.5. The cross section obtained using the (d, 3n) empirical formula of (Kavun, 2020) at 20 MeV is 1820.3 mb which is slightly over predicted than the other theoretical predictions and EXFOR data.

The predictions of EMPIRE data are lower than TALYS data. The experimental data are analogous with TALYS predictions. TALYS data started from 12.2 MeV with 0.0030 mb, which increase up to 24 MeV with 805.3 mb. After 24 MeV, a decrement is observed and at 50 MeV of deuteron energy, the cross section value is 185.75 mb.

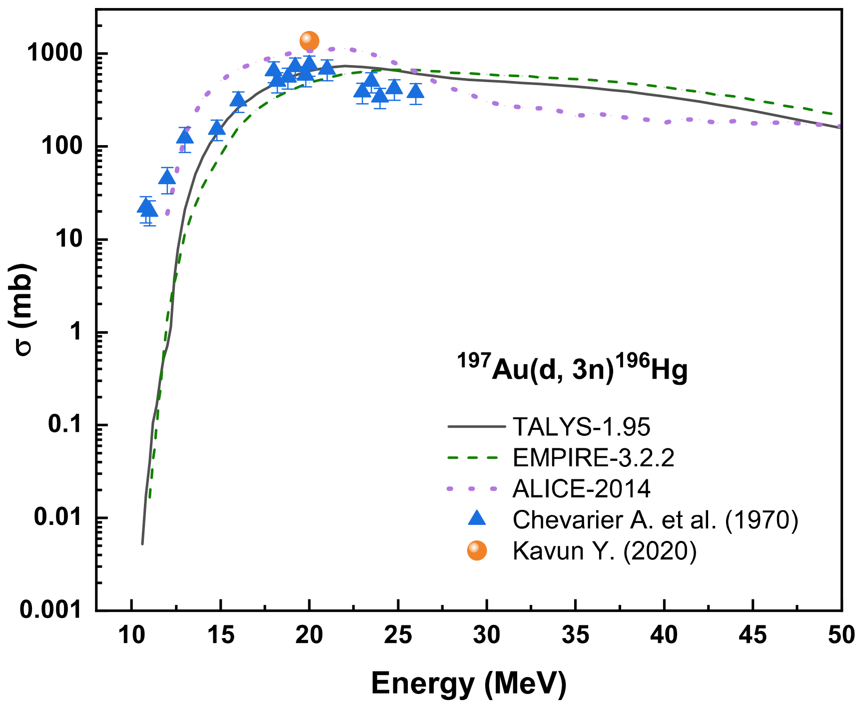

Figure 6.5: Comparison of theoretical predictions with EXFOR data, and the result of Kavun's empirical formula [19] for ^{209}Bi(d, 3n)^{208}Po reaction.

The EMPIRE results started at 13 MeV and took the value of 0.314 mb which increased up to 28 MeV with 434.3 mb. After that, it decreases up to 129.4 mb at 50 MeV. The cross section calculated using the (d, 3n) (Kavun, 2020) empirical formula at 20 MeV is 1820.3 mb. The experimental data by Kelly and Serge (1949) [33] started with 10 mb of value at 12.5 MeV, and increased up to 750 mb at 18.7 MeV. The previously published data of Templeton *et al.* (1947) [34], a cross section value of 1110 mb was obtained at 20 MeV. It is noted that the rest of the cross section for (d, 3n) reaction for three isotopes ^{167}Er, ^{197}Au, and ^{209}Bi are predicted using the theoretical codes from threshold to 50 MeV. Also, it can be realized that the results predicted are following the expected trend from the initial comparison with the available cross section data of the EXFOR data library.

6.4 Conclusion

In this study, the reaction induced by deuteron to produce neutrons has been studied. As discussed in the introduction, the reaction induced by deuteron is important in the fusion reactor technology, accelerators induced reaction mechanism, for determining the accuracy of reaction models and validating nuclear data. Despite many difficulties in defining deuteron induced processes, interest in studying and understanding these types of reactions is increasing.

The (d, 3n) reaction was examined and cross sections were obtained utilizing statistical model codes such as TALYS, EMPIRE, and ALICE. In addition, these data are simulated with the EXFOR data and calculated cross section using (d, 3n) empirical formula developed by Y. Kavun (2020).

Overall, the predicted results by theoretical nuclear codes agree well with the experimental data of the EXFOR. Further, the cross section value obtained utilizing the (d, 3n) empirical formula of Y. Kavun (2020) is more compatible with the TALYS dataset and previously published experimental data retrieved from the EXFOR library. The EXFOR database is in trend with the theoretical predictions. EMPIRE code predicts lower values compared to TALYS and EXFOR data. ALICE code gives well-matched predictions at lower energy with the data of TALYS and EXFOR. As energy increases it gives lower cross section predictions.

As per the obtained results, for ^{112}Cd(d, 3n) reaction, the data of TALYS, EXFOR, and empirical formula of (d, 3n) reaction by Y. Kavun (2020) are more compatible. The prediction of EMPIRE is slightly lower but follows the same trend as the results. The results of ALICE are also well matched at lower energy regions with TALYS, EXFOR, and value of empirical formula but at higher energy regions, the code gives lower predictions compared to TALYS and EXFOR database. For ^{141}Pr(d, 3n)^{140}Nd reaction, the data of TALYS and EXFOR are compatible with each other as well as a value obtained from Kavun's empirical formula is in good agreement with TALYS. Moreover, EMPIRE and ALICE data show the same trend. The more adaptable results were obtained up to 20 MeV for ^{167}Er(d, 3n)^{166}Tm reaction. Further, for ^{197}Au(d, 3n)^{196}Hg reaction, the cross section value calculated from Kavun's empirical formula is slightly higher than theoretical predictions and experimental values. Finally, although a similar situation is valid for the ^{209}Bi(d, 3n)^{208}Po reaction, the theoretical and experimental data are compatible.

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