Chapter 4

Development of New Semi-empirical Formulas

New Semi-empirical mass formulas were developed for the (n, p), (n, 2n), and (n, α) reaction cross-section at 14.5 MeV incident neutron energy by using the literature data available at EXFOR library. The new formulas were derived based on the statistical model, taking into account the Q-value dependence. The results derived from this study were evaluated against other systematic formulas developed previously and compared with experimental data reported in the EXFOR library. The comparison has been done on the basis of statistical model as well as on the asymmetry parameter dependence. The present work offers an alternative to reproduce nuclear data at 14.5 MeV incident neutron energies.

The work presented in this chapter has been published in Peer-Reviewed Journal:
1. A. Hingu, S. Parashari, et. al., Radiat. Phys. Chem., **188**, 109634, (2021). (According to the copyright agreement, the author retains the right to reuse the published work here as a part of this thesis) (Elsevier Copyright Policy). **(I.F.=2.8)**

4.1 Introduction

An understanding of the essential neutron induced reaction cross-sections is of prime interest due to their usability for the design of fusion reactors, dose estimation, rare isotope production, radiation damage studies, advancement of the fission reactors etc. Thus, neutron data around 14 MeV are required with great precision for the (n, p), (n, α), and (n, 2n) reactions [1, 2]. The measurements, calculations and evaluations of these reaction cross-sections, therefore, have been extensively undertaken. Sometimes the data are not directly measured or there are discrepancies among experimental data due to the relative measurements and unavailability of mono-energetic neutron source. Therefore, in such cases, systematic approach or theoretical predictions are applied to estimate neutron-induced reaction cross-sections data more accurately.

Different approaches have been employed to analyze the systematic dependence of neutron-induced reaction cross-sections. The cross-section is commonly expressed by an exponential function, with its argument depending on the number of nucleons in the target nucleus [3].Various authors have used the evaporation model for the exponent function, however, it does not take account of the non-equilibrium particle evaporation for nuclei $\mathrm{A} \geq 6$. A detailed description is also provided in Refs. [3–27] to include both equilibrium and non-equilibrium particle emissions in the semi-empirical approach to understand the systematic dependence of neutron-induced reaction cross-sections. An empirical approach using the principal of detailed balance [11] has shown to provide a better description of the experimental data. Further, a χ^2 test validates the empirical parameters of the systematics. Similar approaches were implicated by several authors [7, 18–23, 28] to study the systematic dependence of (n, p), (n, α), and (n, 2n) reaction cross-sections for the neutron energy around 14 MeV.

In the present work, new semi-empirical formulas around 14.5 MeV incident neutron energy have been developed to calculate and to predict (n, p), (n, α), and (n, 2n) reaction cross-sections within the target mass regions $24 \leq \mathrm{A} \leq 238$ (including both $\mathrm{Z} \leq 45; > 45$) , $26 \leq \mathrm{A} \leq 181$, and $45 \leq \mathrm{A} \leq 238$ (including both even and odd nuclei), respectively. The formulas are based on statistical model including the Q-value dependence. The systematics have been developed by using the data sets from the EXFOR [29] library for the desired reactions between the incident neutron energy range of 14-15 MeV. Maximum number of data points was utilized to enhance the input for the χ^2 test. In cases where multiple measurements exist at the same energy, only the data points with the best fit were considered. The fitting of each data set has been performed by considering a general form of the systematics [7]. A comprehensive comparison has been made between the cross-sections obtained in this study and those calculated using previously established formulas.

4.2 Semi-empirical Formula for (n, p), (n, α) and (n, 2n) Reaction Cross-section

The (n, p), (n, α), or (n, 2n) reaction cross-sections can be written in the basis of statistical model as [7, 11],

$$\sigma_{\rm n,i} = \sigma_{\rm R}\ (\Gamma_{\rm i}/\Gamma_{\rm n}); \qquad ({\rm i = p}, \alpha \ \text{ or } \ 2{\rm n}) \tag{4.1}$$

where, $\sigma_{\rm R}$ is the reaction cross-section for incident neutrons, $\Gamma_{\rm n}$ is the decay width for neutrons, and $\Gamma_{\rm i}$ is the decay width for particle/s emission (either p, α, or 2n). Using the definition given in Eq. (4.1), the semi-empirical formula for (n, p), (n, α), and (n, 2n) reactions can be derived separately. From the principle of detailed balance [11], the decay width for proton can be expressed in the following form,

$$\Gamma_{\rm p} = \frac{(2{\rm S_p}+1){\rm M_p}}{\pi^2\ {\rm h}^2\ \rho_{\rm a}({\rm E_a})} \int_{\rm V_c}^{\rm E_a - B_p - \delta_p} \epsilon_{\rm p}\ \sigma_{\rm c}(\epsilon_{\rm p})\ \rho_{\rm b}({\rm E_b})\ {\rm d}\epsilon_{\rm p}, \tag{4.2}$$

where, $\rm S_p$ is the spin statistical factor, $\rm m_p$ is the mass of proton, $\rho_{\rm a,b}$ are the NLDs with $\rm E_{a,b}$ excitation energies for compound and residual nucleus, $\rm V_c$ is the Coulomb barrier, $\rm B_p$ is the separation energy of the proton, $\delta_{\rm p}$ represents the odd-even character of a nucleus, $\epsilon_{\rm p}$ is the energy of emitted proton, and $\sigma_{\rm c}$ is the the cross-section for reverse process with limiting values at low incident energies as,

$$\sigma_{\rm c}(\epsilon_{\rm n}) = \pi {\rm R}^2,$$

$$\sigma_{\rm c}(\epsilon_{\rm p}) = \pi {\rm R}^2 (1 - \frac{\rm V_p}{\epsilon_{\rm p}}); \ \text{ for } \ \epsilon_{\rm p} > {\rm V_p},$$

$$\sigma_{\rm c}(\epsilon_{\rm p}) = 0; \ \text{ for } \ \epsilon_{\rm p} < {\rm V_p},$$

where, $(1 - {\rm V_p}/\epsilon_{\rm p})$ is the barrier penetration probability for proton under classical limit and $\rm R$ is the nuclear radius. Using the above definitions for $\sigma_{\rm c}$ and level densities as a function of entropy of nucleus, the proton decay width can be written as,

$$\Gamma_{\rm p} = \frac{(2{\rm S_p}+1){\rm M_p}}{\pi^2 {\rm h}^2}\ {\rm R}^2 \int_{\rm V_c}^{\rm E_a - B_p - \delta_p} \epsilon_{\rm p} \Big(1 - \frac{\rm V_p}{\epsilon_{\rm p}}\Big)\ {\rm e}^{-(\epsilon_{\rm p} + {\rm B_p} + \delta_{\rm p})/{\rm T}} {\rm d}\epsilon_{\rm p}. \tag{4.3}$$

The above relation can be further simplifies to,

$$\Gamma_{\rm p} \approx \frac{(2{\rm S_p}+1){\rm M_p}}{\pi^2 {\rm h}^2}\ {\rm R}^2\ {\rm T}^2 \Big(1 - \frac{\rm V_p}{\epsilon_{\rm p}}\Big) + {\rm e}^{-({\rm V_p} + {\rm B_p} + \delta_{\rm p})/{\rm T}}. \tag{4.4}$$

Similarly, the neutron decay width can be expressed as,

$$\Gamma_{\rm n} \approx \frac{(2{\rm S_n}+1){\rm M_p}}{\pi^2 {\rm h}^2}\ {\rm R}^2\ {\rm T}^2\ {\rm e}^{-({\rm B_n} + \delta_{\rm n})/{\rm T}}. \tag{4.5}$$

4.2.1 Semi-empirical Formula for (n, p) Reaction Cross-section

By using Eq. (4.4) and (4.5) into Eq. (4.1), the (n, p) reaction cross-section can be written as,

$$\sigma_{\mathrm{n,p}} = \sigma_{\mathrm{R}} \frac{(2\mathrm{S_n}+1)}{(2\mathrm{S_n}+1)} \left(\frac{\mathrm{M_p}}{\mathrm{M_n}}\right) \left(1 - \frac{\mathrm{V_p}}{\epsilon_{\mathrm{p}}}\right) \mathrm{e}^{(\mathrm{Q_{n,p}} - \mathrm{V_p})/\mathrm{T}}, \tag{4.6}$$

where, $\mathrm{T} = (\mathrm{E_n}/\mathrm{a})^{1/2}$ MeV is the nuclear temperature with $\mathrm{E_n}$ being the incident neutron energy and level density parameter $\mathrm{a} = (\mathrm{A}/15)\ \mathrm{MeV}^{-1}$, $\sigma_{\mathrm{R}} = \pi \mathrm{r}_0^2(1 + \mathrm{A}^{1/3})$ is the formation cross-section with $\mathrm{r_0} = 1.4$ fm, and $\mathrm{Q_{n,p}} = \mathrm{B_n} - \mathrm{B_p} + \delta_{\mathrm{n}} - \delta_{\mathrm{p}}$ is the effective Q-value of the reaction, which can also be written from the semi-empirical mass formula (symbols have their usual meanings) as,

$$\mathrm{Q_{n,p}} = \frac{\mathrm{a_c}(2\mathrm{Z}-1)}{\mathrm{A}^{1/3}} - \frac{4\mathrm{a_a}(\mathrm{A}-2\mathrm{Z}+1)}{\mathrm{A}}.$$

Now the final form of the (n, p) reaction cross-sections can be written as,

$$\sigma_{\mathrm{n,p}} = \sigma_{\mathrm{R}} \frac{(2\mathrm{S_n}+1)}{(2\mathrm{S_n}+1)} \left(\frac{\mathrm{M_p}}{\mathrm{M_n}}\right) \left(1 - \frac{\mathrm{V_p}}{\epsilon_{\mathrm{p}}}\right) \exp\left[\frac{\mathrm{a_c}(2\mathrm{Z}-1)}{\mathrm{TA}^{1/3}} - \frac{4\mathrm{a_a}(\mathrm{A}-2\mathrm{Z}+1)}{\mathrm{TA}} - \frac{\mathrm{V_p}}{\mathrm{T}}\right]. \tag{4.7}$$

4.2.2 Semi-empirical Formula for (n, α) Reaction Cross-section

The Q-value for this reaction can be written as,

$$\mathrm{Q}_{\mathrm{n},\alpha} = \mathrm{a_1} + \mathrm{a_c}\left[\frac{\mathrm{Z}^2}{\mathrm{A}^{1/3}} - \frac{(\mathrm{Z}-2)^2}{(\mathrm{A}-3)^{1/3}} - 2.519\right] + \mathrm{a_a}\left[\frac{(\mathrm{A}-2\mathrm{Z})^2}{\mathrm{A}} - \frac{(\mathrm{A}-2\mathrm{Z}+1)^2}{(\mathrm{A}-3)}\right], \tag{4.8}$$

where, $\mathrm{a_c}$ and $\mathrm{a_a}$ are the Coulomb and asymmetry parameters and $\mathrm{a_1}$ is the constant in place of the other constant terms of semi-empirical mass formula. The (n, α) reaction cross-section can be written as,

$$\sigma_{\mathrm{n},\alpha} = \sigma_{\mathrm{R}} \left(\frac{\mathrm{M}_\alpha}{\mathrm{M_n}}\right) \exp\left(\mathrm{a_0} + \frac{\mathrm{Q}_{\mathrm{n},\alpha}}{\mathrm{T}} - \frac{\mathrm{V}_\alpha}{\mathrm{T}}\right), \tag{4.9}$$

where, $\mathrm{a_0} = \ln \mathrm{c}(1 - \mathrm{V}_\alpha/\epsilon_\alpha)$, with $\mathrm{c} = (2\mathrm{S}_\alpha + 1)/(2\mathrm{S_n} + 1)$. The quantity $(1 - \mathrm{V}_\alpha/\epsilon_\alpha)$ is the barrier penetration probability for the alpha particle of energy ϵ_α, V_α is the Coulomb barrier of the alpha particle, $\mathrm{T} = (\mathrm{E_n}/\epsilon_\alpha)$ is the nuclear temperature, $\mathrm{a} = (\mathrm{A}/15)\ \mathrm{MeV}^{-1}$ is the level density parameter, σ_{R} is the reaction formation cross-section, and M_α and $\mathrm{M_n}$ are the mass of alpha particle and neutron, respectively.

4.2.3 Semi-empirical Formula for (n, 2n) Reaction Cross-section

The (n, 2n) reaction cross-section can be written as,

$$\sigma_{\mathrm{n,2n}} = \sigma_{\mathrm{R}} \frac{(2\mathrm{S}_{\mathrm{2n}}+1)}{(2\mathrm{S}_{\mathrm{n}}+1)} \Big(\frac{\mathrm{M}_{\mathrm{2n}}}{\mathrm{M}_{\mathrm{n}}}\Big) \mathrm{e}^{\mathrm{Q}_{\mathrm{n,2n}}/\mathrm{T}}, \tag{4.10}$$

where, $\mathrm{Q}_{\mathrm{n,p}} = \mathrm{B}_{\mathrm{n}} - \mathrm{B}_{\mathrm{2n}} + \delta_{\mathrm{n}} - \delta_{\mathrm{2n}}$ is the effective Q-value of the reaction and rest of the symbols have their meanings for incoming and outgoing neutrons similar to Eq. (4.6). The Q-value of the (n, 2n) reaction can be given by semi-empirical mass formula as,

$$\mathrm{Q}_{\mathrm{n,2n}} = \mathrm{a}_1 + \mathrm{a}_{\mathrm{c}} \Big[\frac{\mathrm{Z}^2}{\mathrm{A}^{1/3}} - \frac{\mathrm{Z}^2}{(\mathrm{A}-1)^{1/3}}\Big] + \mathrm{a}_0 \Big[\frac{(\mathrm{A}-2\mathrm{Z})^2}{\mathrm{A}} - \frac{(\mathrm{A}-2\mathrm{Z}+1)^2}{\mathrm{A}-1}\Big].$$

Thus, the (n, 2n) reaction cross-section can be written as,

$$\begin{aligned} \sigma_{\mathrm{n,2n}} = \sigma_{\mathrm{R}} \frac{(2\mathrm{S}_{\mathrm{2n}}+1)}{(2\mathrm{S}_{\mathrm{n}}+1)} \Big(\frac{\mathrm{M}_{\mathrm{2n}}}{\mathrm{M}_{\mathrm{n}}}\Big) \exp\Bigg(\mathrm{a}_1 + \mathrm{a}_{\mathrm{c}} \Big[\frac{\mathrm{Z}^2}{\mathrm{A}^{1/3}} - \frac{\mathrm{Z}^2}{(\mathrm{A}-1)^{1/3}}\Big] \\ + \mathrm{a}_0 \Big[\frac{(\mathrm{A}-2\mathrm{Z})^2}{\mathrm{A}} - \frac{(\mathrm{A}-2\mathrm{Z}+1)^2}{\mathrm{A}-1}\Big]\Bigg), \end{aligned} \tag{4.11}$$

where, $\mathrm{T} = (\mathrm{E}_{\mathrm{n}}/\mathrm{a})^{1/2}$ MeV is the nuclear temperature, $\mathrm{a} = (\mathrm{A}/15)\ \mathrm{MeV}^{-1}$ is the NLD parameter and E_{n} is the incident neutron energy. The formulas presented in Eq. (4.7) and (4.11) were parameterized to establish a new systematic by fitting experimental data available for various nuclei.

4.3 Fitting Procedure for Systematics Parameters

A general form of the systematics was used in Eq. (4.12) for the fitting of (n, p), (n, α), and (n, 2n) reaction experimental data, following the Legendre least square method. The experimental cross-section values at 14.5 MeV for even and odd nuclei were taken from EXFOR [29] library as primary input. Other input parameters such as atomic number, masses and NLD parameters were used appropriately. An exponential function Y having the following form,

$$\mathrm{Y} = \alpha \exp(\beta \mathrm{X} + \gamma \mathrm{X}^2), \tag{4.12}$$

was used to calculate find the fitting parameters, α, β, and γ. Where, $\mathrm{Y} = \sigma/(\mathrm{A}^{1/3}+1)$ and $\mathrm{X} = (\mathrm{A}-2\mathrm{Z})/\mathrm{A}$ is called the asymmetric term. The fitting has been performed using the neutron data for the (n, p), (n, α), and (n, 2n) reactions, available at EXFOR library. The data have been categorized into two groups for each reaction: according to atomic number Z ($\mathrm{Z} \leq 45$ & $\mathrm{Z} > 45$) for the (n, p) reaction, and according to their even-odd characteristics for the (n, 2n) reaction.

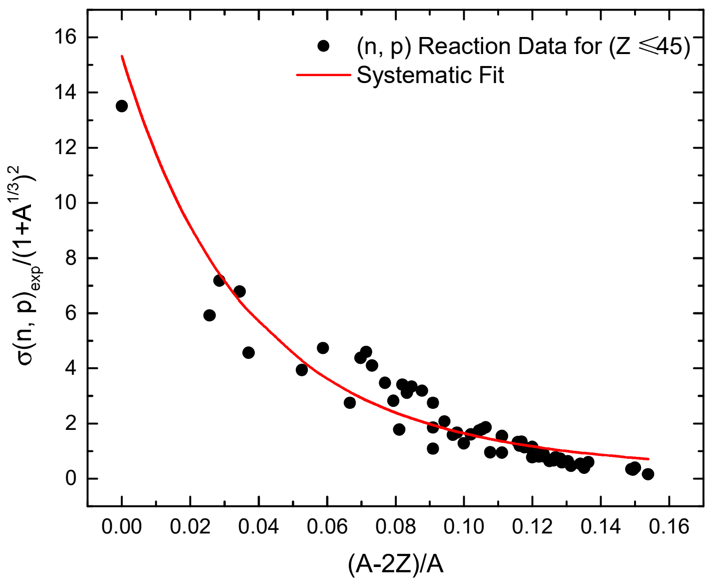

Fig. 4.1: Systematic fitting of the $(\mathrm{n,p})$ reaction cross-sections for nuclei $\mathrm{Z} \leq 45$ at the neutron energy of 14.5 MeV.

4.3.1 The (n, p) Reaction Cross-section Systematics

A good fit for the cross-section data obtained by the present formula satisfying both the conditions of 'Z', is given by,

$$\sigma_{\mathrm{n,p}}/(1+\mathrm{A}^{1/3})^2 = \alpha \exp\left[\beta\frac{(\mathrm{A}-2\mathrm{Z})}{\mathrm{A}} + \gamma\frac{(\mathrm{A}-2\mathrm{Z})^2}{\mathrm{A}^2}\right], \tag{4.13}$$

where, α, β, and γ are the fitting parameters, with the values,

$$\alpha = 15.32, \quad \beta = -26.73, \quad \gamma = 44.19; \quad \text{for } \mathrm{Z} \leq 45,$$

$$\alpha = 1.67, \quad \beta = 2.15758, \quad \gamma = -93.1318; \quad \text{for } \mathrm{Z} > 45.$$

By using the obtained values of parameters, the systematics for $(\mathrm{n,p})$ reaction at 14.5 MeV energy for nuclei with $\mathrm{Z} \leq 45$ and $\mathrm{Z} > 45$, are plotted in Fig. (4.1) and (4.2), respectively.

4.3.2 The (n, α) Reaction Cross-section Systematics

A good fit has been obtained for the (n,α) reaction at 14.5 MeV energy by using the following form of the systematics,

$$\sigma_{\mathrm{n},\alpha} = \mu(1+\mathrm{A}^{1/3})^2 \exp[\nu(\mathrm{A}-2\mathrm{Z}-\delta)/\mathrm{A}], \tag{4.14}$$

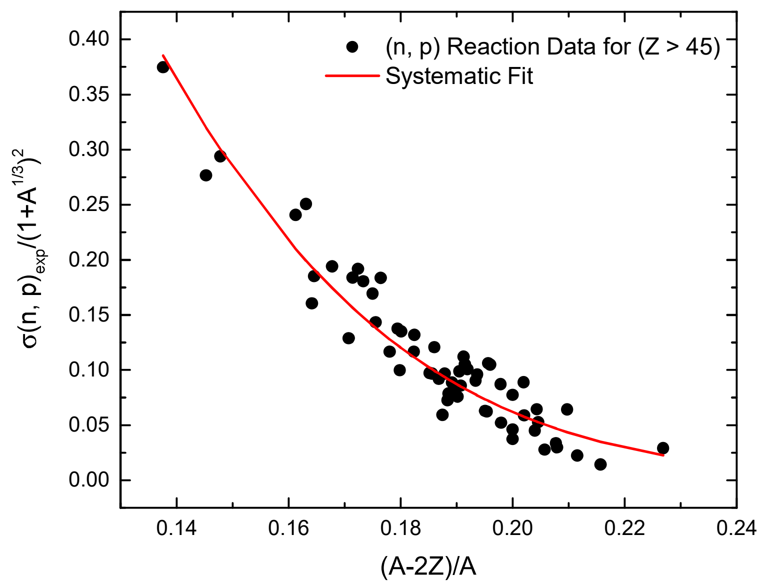

Fig. 4.2: Systematic fitting of the $(\mathrm{n,p})$ reaction cross-sections for nuclei $\mathrm{Z} > 45$ at the neutron energy of 14.5 MeV.

where, μ and ν are the fitting parameters and δ takes care the odd-even character of the nuclei. The fitting parameters have the following values,

$$\mu = 30.59,\ \nu = -35.75,\ \delta = 0.$$

The systematics for the (n,α) reaction at 14.5 MeV energy by using the obtained values of the parameters is plotted in the Fig. (4.3).

4.3.3 The (n, 2n) Reaction Cross-section Systematics

A good fit is obtained for the cross-section data for (n, 2n) reaction at 14.5 MeV by using the systematics given in Eq. (4.11) as,

$$\sigma_{\mathrm{n,2n}}/(1+\mathrm{A}^{1/3})^2 = \psi \exp\left[\phi\frac{(\mathrm{A}-2\mathrm{Z})}{\mathrm{A}} + \Delta\frac{(\mathrm{A}-2\mathrm{Z})^2}{\mathrm{A}^2}\right], \tag{4.15}$$

where the fitting parameters derived are presented for odd-A and even-A nuclei, respectively, as follows:

$$\psi = 1.344, \quad \phi = 40.53, \quad \Delta = -116.5; \quad \text{for even} - \mathrm{A},$$

$$\psi = 4.397, \quad \phi = 27.77, \quad \Delta = -82.26; \quad \text{for odd} - \mathrm{A}.$$

The systematics for the $(\mathrm{n},2\mathrm{n})$ reaction at 14.5 MeV energy by using the obtained values of the parameters are plotted in the Fig. (4.4) and (4.5) for even-A and

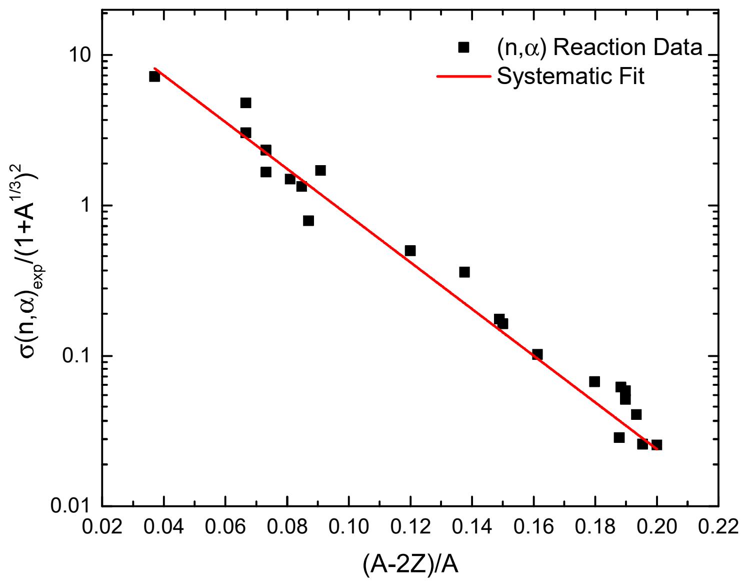

Fig. 4.3: Systematic fitting of the (n, α) reaction cross-sections at the neutron energy of 14.5 MeV.

odd-A nuclei, respectively.

4.4 Results and Discussion

The goodness of the fit has been determined by using the quantity $\mathrm{F/n}$, proposed by Csikai et al., [1, 26]. The $\mathrm{F/n}$ presents the comparison among various systematic formulas, where F is given as,

$$\mathrm{F} = \sum_{\mathrm{k}=1}^{\mathrm{n}} \left(|\sigma_{\mathrm{k}}^{\mathrm{exp}} - \sigma_{\mathrm{k}}^{\mathrm{cal}}| \right) / \sigma_{\mathrm{k}}^{\mathrm{cal}}, \tag{4.16}$$

here, σ^{exp} and σ^{cal} are the experimental cross-section from EXFOR [29] and calculated cross-section from systematic formula, respectively, and 'n' represents the number of data points employed in the fitting of the systematics. A ratio ($\sigma_{\mathrm{exp}}/\sigma_{\mathrm{cal}}$) has been derived to assess the relative discrepancy between the observed cross-sections (σ_{exp}) and those predicted by the current systematics (σ_{cal}). The relative error provides the accuracy of the calculated cross-sections.

The $\mathrm{F/n}$ parameter has been evaluated for each systematic formula in this work and benchmarked against previously developed formulas for the (n, p), (n, α), and (n, 2n) reaction cross-sections at a neutron energy of 14.5 MeV, as shown in Tables 4.1, 4.2, and 4.3, respectively. Fitting parameters for each reaction are detailed in Table 4.4 based on their mass ranges. A comparative analysis of neutron-induced reaction cross-sections at 14.5 MeV, calculated using

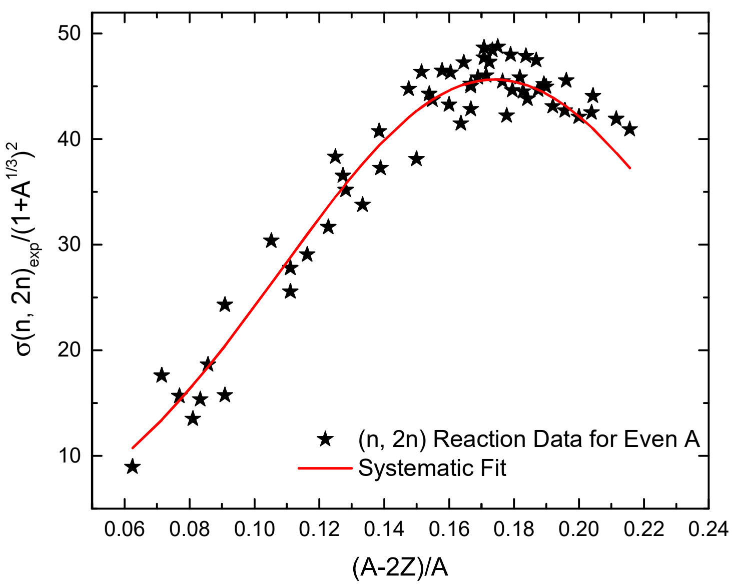

Fig. 4.4: Systematic fitting of the $(\mathrm{n}, 2\mathrm{n})$ reaction cross-sections for even-A nuclei at the neutron energy of 14.5 MeV.

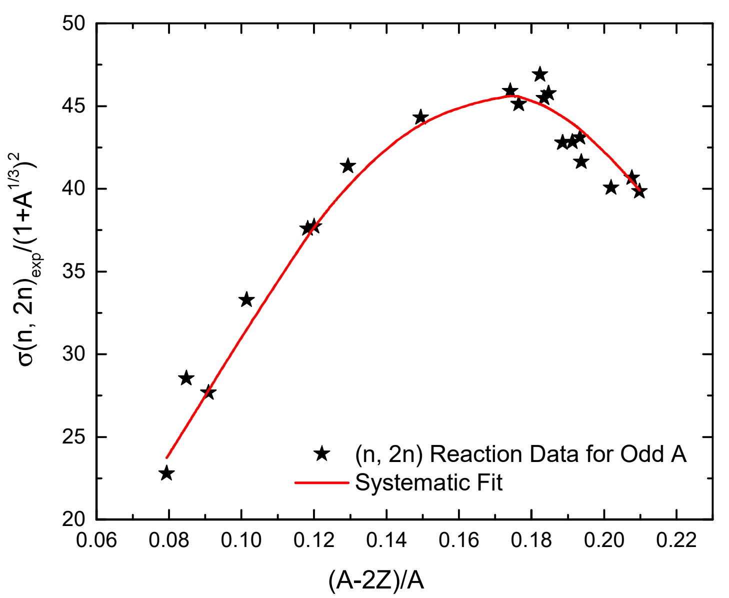

Fig. 4.5: Systematic fitting of the $(\mathrm{n}, 2\mathrm{n})$ reaction cross-sections for odd-A nuclei at the neutron energy of 14.5 MeV.

various systematics, experimental data, and the current formulas, is detailed in Appendix B, Tables 1 through 5. A detailed discussion of each systematic formula is provided in the subsequent subsections.

4.4.1 The (n, p) Reaction

The (n, p) reaction cross-sections predicted by semi-empirical formulas (4.13) for the mass regions $24 \leq \mathrm{A} \leq 103$ (for $\mathrm{Z} \leq 45$) and $108 \leq \mathrm{A} \leq 238$ (for $\mathrm{Z} > 45$) are listed in Appendix Tables 1 and 2, respectively. The calculated cross-sections are compared with the experimentally measured data [29] as well as with the systematics proposed by other authors [3, 7, 8, 14, 16, 17, 25, 27, 28] for the (n, p) reaction cross-sections at 14.5 MeV neutron energy. The predicted (n, p) reaction cross-sections using the current systematics are in good agreement with the experimental data. However, a general discrepancy between the current results and experimental measurements is also noted in the (n, p) reactions for certain nuclei $^{39}\mathrm{K}$, $^{42}\mathrm{Ca}$, $^{47}\mathrm{Ti}$, and $^{56}\mathrm{Fe}$. The current results are consistent with the previously developed systematics. The present systematic formulas with the fitting parameters are given in Table 4.1. It is also evident from Table 4.1 that the current systematic exhibits better 'F/n' relative to those presented in the table. The relative error between the current results and experimental data is also assessed, with the corresponding data depicted in Fig. (4.6). The relative error was found to be between 0.6 and 1/0.6. Based upon the discussion above, it can be said that the new semi-empirical formulas for (n, p) reaction at 14.5 incident neutron energy is quite satisfactory in estimating the cross-sections.

4.4.2 The (n, α) Reaction

The (n, α) reaction cross-sections were calculated for the mass region $26 \leq \mathrm{A} \leq 181$ using the present systematic formula (Eq. (4.14)). The results were compared in Appendix Table 3 with the experimental data [29] and the predictions of the previously developed systematics [3, 7, 16, 17, 21, 25, 26]. It is evident from the data presented in the Table that the current results are consistent with the experimental data within minor uncertainties. The trend of data fitting by the expressions given by Levkovski [3], Ali-Tahar [17] and Kasugai et al. [25], confirms the straight line trend for the asymmetry parameters like, $(\mathrm{N}-\mathrm{Z})/\mathrm{A}$ and $(\mathrm{N}-\mathrm{Z}+1)/\mathrm{A}$. The other formulas from Forrest [16] and Csikai et al. [26] contains additional terms in the exponential function, which rather improves the fitting. However, the results obtained in this study (with $\mathrm{F/n} = 0.27$) are significantly better than those from prior research. The relative error in the current results and the experimental data were evaluated and plotted in Fig. (4.7), and is found to be within the limit of $0.6 - 1/0.6$, which shows a good accuracy of the present (n, α) systematics.

Table 4.1: Systematic formulas proposed by different authors for (n, p) reactions.

Author	Formula for $\sigma_{n,p}$ (mb)	Mass region	n	F/n
Levkovski [3]	$\sigma_{n,p} = 50.21(A^{1/3}+1)^2 \exp\left(-\frac{33.80(N-Z)}{A}\right)$	$40 \leq A \leq 209$	36	0.37
Forrest [16]	$\sigma_{n,p} = 900(A^{1/3}+1)^2 \exp\left(-49.27\frac{(N-Z)}{A} + 197.1\frac{(N-Z)^2}{A^2} - 0.45A^{1/2}\right)$	$40 \leq A \leq 187$	33	0.77
Ait-Tahar [17]	$\sigma_{n,p} = 90.68(A^{1/3}+1)^2 \exp\left(-\frac{34.48(N-Z+1)}{A}\right)$	$40 \leq A \leq 187$	33	0.77
Kasugai et al. [25]	$\sigma_{n,p} = 1264(N-Z+1) \exp\left(-\frac{46.63(N-Z+1)}{A}\right)$	$28 \leq A \leq 187$	33	0.32
Doczi et al. [27]	$\sigma_{n,p} = 18.12(A^{1/3}+1)^2 \exp\left(-19.61\left(\frac{(N-Z)}{A} + \frac{(N-Z)^2}{A^2}\right)\right)$	$28 \leq A \leq 209$	36	0.56
Bychkov [14]	$\sigma_{n,p} = 7.06\pi r_0^2(A^{1/3}+1)^2 \exp\sqrt{\frac{a}{E_n}}\left(\frac{0.58(Z-1)}{A^{1/3}} - \frac{50(N-Z+1)}{A} - 3.26\right)$	$28 \leq A \leq 209$	100	
J. Luo [28]	$\sigma_{n,p} = 62.98(A^{1/3}+1)^2 \exp\left(-34.45\frac{(N-Z)}{A}\right)$	$46 \leq A \leq 196$	36	0.31
Habbani et al. [7]	$\sigma_{n,p} = 60.34(A^{1/3}+1)^2 \exp\left(-34.44\frac{(N-Z+1)}{A}\right)$	$28 \leq A \leq 208$ (even-A)	23	0.72
	$\sigma_{n,p} = 20.91(A^{1/3}+1)^2 \exp\left(-29.53\frac{(N-Z)}{A}\right)$	$29 \leq A \leq 209$ (odd-A)	13	0.58
Broeders and	$\sigma_{n,p} = 50.093(A^{1/3}+1)^2 \exp\left(A^{0.5}(-4.4785\frac{(N-Z+1)}{A} + 0.047174Z/A^{1/3} - 0.27407)\right)$	$Z \leq 50$	17	0.31
Konobeye [8]	$\sigma_{n,p} = 50.093(A^{1/3}+1)^2 \exp\left(A^{0.75718}(-0.61348\frac{(N-Z+1)}{A} + 0.1511)\right)^3$	$Z > 50$	19	0.44
Present	$\sigma_{n,p} = 15.32(A^{1/3}+1)^2 \exp\left(-26.73(N-Z)/A + 44.19(N-Z)^2/A^2\right)$	$24 \leq A \leq 103$ (for $Z \leq 45$)	65	0.30
	$\sigma_{n,p} = 1.67(A^{1/3}+1)^2 \exp\left(2.158(N-Z)/A - 93.13(N-Z)^2/A^2\right)$	$108 \leq A \leq 238$ (for $Z > 45$)	68	0.23

Table 4.2: Systematic formulas proposed by different authors for (n,α) reactions.

Author	Formula for $\sigma_{\mathrm{n},\alpha}$ (mb)	Mass region	n	F/n
Levkovski [3]	$\sigma_{\mathrm{n},\alpha} = 16.55(\mathrm{A}^{1/3}+1)^2 \exp\Big(-31.26(\mathrm{N}-\mathrm{Z})/\mathrm{A}\Big)$	$31 \leq \mathrm{A} \leq 202$	12	0.30
Forrest [16]	$\sigma_{\mathrm{n},\alpha} = 24.71(\mathrm{A}^{1/3}+1)^2 \exp\Big(-19.77(\mathrm{N}-\mathrm{Z})/\mathrm{A} + 13.82(\mathrm{N}-\mathrm{Z})^2/\mathrm{A}^2 - 0.0248\mathrm{A}\Big)$	$20 \leq \mathrm{Z} \leq 50$	7	0.47
	$\sigma_{\mathrm{n},\alpha} = 11.44(\mathrm{A}^{1/3}+1)^2 \exp\Big(-16.32(\mathrm{N}-\mathrm{Z})/\mathrm{A} - 0.014\mathrm{A}\Big)$	$50 \leq \mathrm{Z} \leq 82$	7	0.26
Ali-Tahar [17]	$\sigma_{\mathrm{n},\alpha} = 31.66(\mathrm{A}^{1/3}+1)^2 \exp\Big(-32.75(\mathrm{N}-\mathrm{Z}+1)/\mathrm{A} - 0.014\mathrm{A}\Big)$	$40 \leq \mathrm{A} \leq 188$	12	0.40
Kasugai et al. [25]	$\sigma_{\mathrm{n},\alpha} = 227.86 \exp\Big(-24.66(\mathrm{N}-\mathrm{Z})/\mathrm{A}\Big)$	$19 \leq \mathrm{A} \leq 187$	12	0.38
Konobeye et al. [21]	$\sigma_{\mathrm{n},\alpha} = 53.066(\mathrm{A}^{1/3}+1)^2 \exp\Big(-209.11\,\mathrm{S}^2 + 8.4723\,\mathrm{P} - 0.19253\,\mathrm{Z}/\mathrm{A}^{1/3} - 0.96249\Big);\quad \mathrm{Z} \leq 50$	$40 \leq \mathrm{A} \leq 209$	7	0.15
	$\sigma_{\mathrm{n},\alpha} = 53.066(\mathrm{A}^{1/3}+1)^2 \Big(-1.6462\,\mathrm{P} + 0.39951\Big)^3;\quad \mathrm{Z} > 50$ $\mathrm{S} = (\mathrm{N}-\mathrm{Z}+1)/\mathrm{A};\quad \mathrm{P} = (\mathrm{N}-\mathrm{Z}+0.5)/\mathrm{A}$	$40 \leq \mathrm{A} \leq 209$	6	0.41
Csikai et al. [26]	$\sigma_{\mathrm{n},\alpha} = 15.07(\mathrm{A}^{1/3}+1)^2 \exp\Big(-25.98\big((\mathrm{N}-\mathrm{Z})/\mathrm{A} + (\mathrm{N}-\mathrm{Z})^2/\mathrm{A}^2\big)\Big)$	$19 \leq \mathrm{A} \leq 202$	12	0.31
Habbani et al.[7]	$\sigma_{\mathrm{n},\alpha} = 3.6(\mathrm{A}^{1/3}+1)^2 \exp\Big(-25(\mathrm{N}-\mathrm{Z}-3)/\mathrm{A}\Big)$	$26 \leq \mathrm{A} \leq 238$ (even-A)	7	0.38
	$\sigma_{\mathrm{n},\alpha} = 35(\mathrm{A}^{1/3}+1)^2 \exp\Big(-37.714(\mathrm{N}-\mathrm{Z})/\mathrm{A}\Big)$	$27 \leq \mathrm{A} \leq 209$ (odd-A)	6	0.26
Present	$\sigma_{\mathrm{n},\alpha} = 30.59(\mathrm{A}^{1/3}+1)^2 \exp\Big(-35.75(\mathrm{N}-\mathrm{Z})/\mathrm{A}\Big)$	$26 \leq \mathrm{A} \leq 181$	23	0.27

Table 4.3: Systematic formulas proposed by different authors for (n, 2n) reactions.

Author	Formula for $\sigma_{n,2n}$ (mb)	Mass region	n	F/n
Chatterjee [12]	$\sigma_{n,2n} = 31.39(A^{1/3}+1)^2 \exp\left(\frac{1.706(N-Z)}{A}\right)$	$45 \leq A \leq 238$	49	0.17
Lu and Fink [13]	$\sigma_{n,2n} = 45.76(A^{1/3}+1)^2\left[1-7.372\exp\left(-\frac{32.21(N-Z+1)}{A}\right)\right]$	$28 \leq Z \leq 82$	45	0.10
J. Luo [28]	$\sigma_{n,2n} = 0.0226(A^{1/3}+1)^2\exp\left(\frac{133.86(N-Z)}{A}-\frac{779.47(N-Z)^2}{A^2}+\frac{1500.51(N-Z)^3}{A^3}\right)$	$23 \leq A \leq 209$	50	0.11
Bychkov [14]	$\sigma_{n,2n} = 8.7(A+100)\left[1-0.88\exp\left(-\frac{7.95(N-Z)}{A}\right)\right]$	$45 \leq A \leq 238$	49	0.16
Habbani et al. [7]	$\sigma_{n,2n} = 23.53(A^{1/3}+1)^2\exp\left(3.50\frac{(N-Z)}{A}\right)$	$45 \leq A \leq 209$ (odd-A)	10	0.08
	$\sigma_{n,2n} = 20.82(A^{1/3}+1)^2\exp\left(3.76\frac{(N-Z+1)}{A}\right)$	$48 \leq A \leq 238$ (even-A)	39	0.19
Konobeye and Korovin [23]	$\sigma_{n,2n} = 53.066(A^{1/3}+1)^2\left[1-\frac{43.5Q_N^2-2Q_N^3}{A^{1/3}S^3}\right]$ $S = -11.068+270.15[(N-Z+2.35)/A]-735.93[(N-Z+2.35)/A]^2+\alpha_5\frac{1}{A^{3/4}}$ $Q_N = 13.848-31.457[(N-Z+0.5)/A]$, even-N $Q_N = 9.846-19.558[(N-Z+0.5)/A]$, odd-N	$40 \leq A \leq 209$	49	0.16
Present	$\sigma_{n,2n} = 1.344(A^{1/3}+1)^2\exp\left(40.53(N-Z)/A-116.5(N-Z)^2/A^2\right)$	$48 \leq A \leq 238$ (even-A)	79	0.11
	$\sigma_{n,2n} = 4.39(A^{1/3}+1)^2\exp\left(27.77(N-Z)/A-82.26(N-Z)^2/A^2\right)$	$45 \leq A \leq 209$ (odd-A)	39	0.08

Table 4.4: Fitting parameters for (n, p), (n, α) and (n, 2n) reactions.

Parameter	(n, p) Reaction		Parameter	(n, α) Reaction	Parameter	(n, 2n) Reaction	
	$Z \leq 45$	$Z > 45$				odd-A	even-A
α	15.32	1.67	μ	30.59	ψ	4.397	1.344
β	-26.73	2.158	ν	-35.75	ϕ	27.77	40.53
γ	44.19	-93.13	δ	0	Δ	-82.26	-116.5

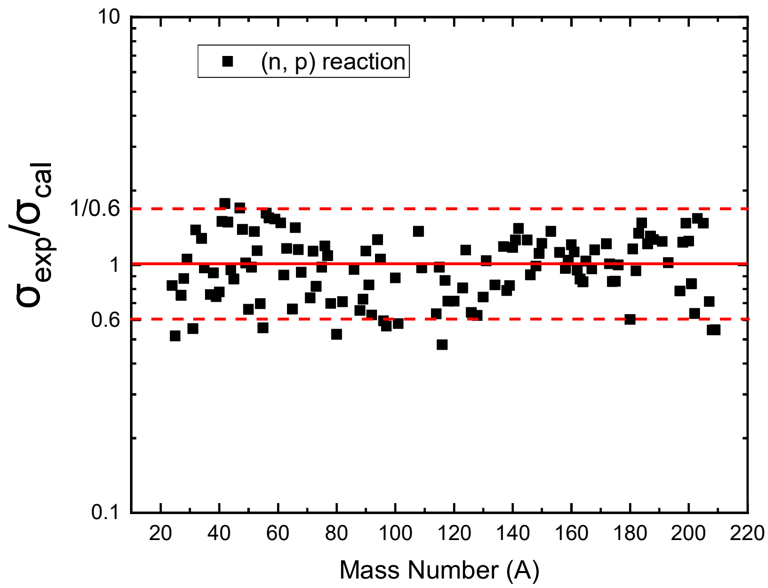

Fig. 4.6: Ratio of the experimental and calculated (n, p) reaction cross-sections for the nuclei within the range $24 \leq A \leq 238$.

4.4.3 The (n, 2n) Reaction

The (n, 2n) reaction cross-sections were calculated using the present semi-empirical formulas for both odd and even-A nuclei within the mass region of $45 \leq A \leq 238$. The current results are compared with the experimental as well as with the systematics from other authors [7, 12–14, 23, 28]. The comparison is shown in Appendix Tables 4 and 5. Among the other authors, the formula proposed by Habbani and Osman [7] is based on the statistical model, on the other hand, formula given by Bychkov et al. [14] is based on the asymmetric dependence. The data presented in the Table demonstrate that the current results are consistent with the experimental data, however, a disagreement can be observed in the cases of ^{92}Mo, ^{98}Ru, ^{124}Sn, ^{148}Sm, ^{154}Sm, ^{176}Yb, ^{192}Os, and ^{232}Th nuclei. The relative error is plotted in Fig. (4.8) and is found within $0.7 - 1/0.7$. The $F/n = 0.11$ and 0.08 for even and odd-A nuclei, respectively, is also better than the previously developed systematics.

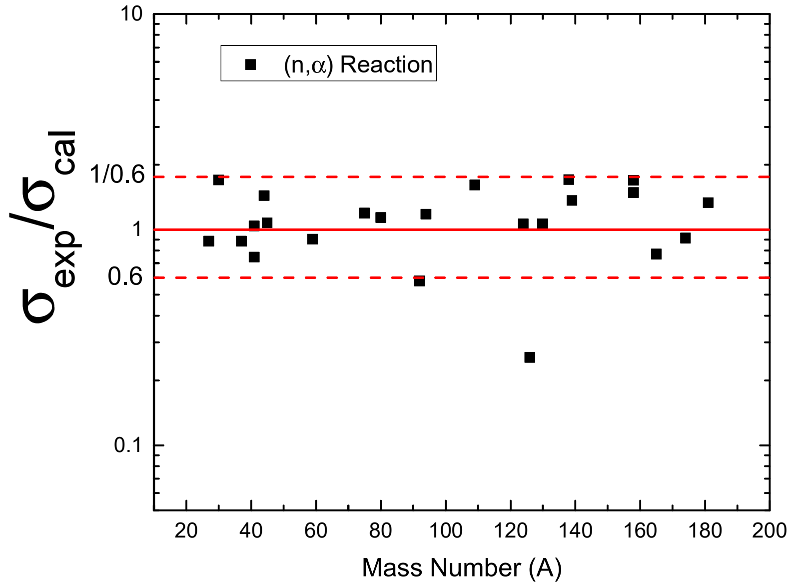

Fig. 4.7: Ratio of the experimental and calculated (n, α) reaction cross-sections for the nuclei within the range $26 \leq \mathrm{A} \leq 181$.

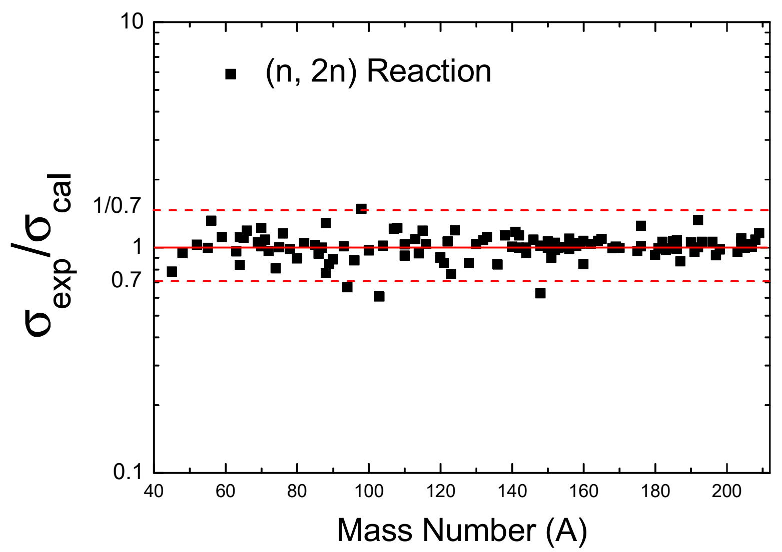

Fig. 4.8: Ratio of the experimental and calculated $(\mathrm{n}, 2\mathrm{n})$ reaction cross-sections for the nuclei within the range $45 \leq \mathrm{A} \leq 238$.

4.4.4 Validation of the Systematic Formulas

To validate the systematic formulas, we computed neutron-induced reaction cross-section for Ni isotopes across all possible channels using the systematic formulas from various authors [3, 7, 8, 12–14, 16, 17, 21, 25–28, 30] and the results were compared to experimental data extracted from the EXFOR database at an energy of 14.5 MeV. The cross-sections calculated for the (n, p), (n, α) and $(\mathrm{n}, 2\mathrm{n})$ reactions are listed in Tables 4.5, 4.6 and 4.7 respectively. The (n, p) reaction on the Ni isotopes $[^{\mathrm{A}}\mathrm{Ni}(\mathrm{n}, \mathrm{p})^{\mathrm{A}}\mathrm{Co}]$ results in Co residues for a particular mass number A. The calculated results are presented in Table 4.5, along with the experimental data from EXFOR. The results shown in Table 4.5 indicate that the cross-sections calculated using the systematic formulas from various authors are consistent with each other and effectively correspond to the the experimental data, except for the results calculated by Forrest [16]. However, the results from Doczi et al. [27] and Habbani et al. [7] showed the greatest consistency with the experimental data from EXFOR. In the case of the (n, α) reaction, there are three Ni isotopes that produce Fe residue. The results obtained from the evaluation are presented in Table 4.6. The systematic formulas presented in Table 4.2 accurately reproduce literature data for (n, α) reactions to a satisfactory extent. The possible $(\mathrm{n}, 2\mathrm{n})$ reaction in Ni isotopes are $^{58}\mathrm{Ni}(\mathrm{n}, 2\mathrm{n})^{57}\mathrm{Ni}$ and $^{61}\mathrm{Ni}(\mathrm{n}, 2\mathrm{n})^{60}\mathrm{Ni}$. All other Ni isotopes undergo $(\mathrm{n}, 2\mathrm{n})$ reactions to produce stable Ni isotopes. The results for the $(\mathrm{n}, 2\mathrm{n})$ reaction are detailed in Table 4.7.

Table 4.5: The cross-sections for the (n, p) reaction on Ni isotopes calculated by utilizing the systematic formulas provided in the Table 4.1.

A	$\sigma_{(\mathrm{n,p})}$ (mb) around 14.5 MeV								
	Levkovski	Forrest	Ait-Tahar	Kasugai et al	Doczi et al	Habbani et al.	Broeders and Konobeyev	J. Luo	Hingu et al.	EXFOR data
58	371.39	160.33	361.56	339.93	213.59	241.09	359.94	455.52	152.40	278 ± 12
60	127.41	59.89	123.78	129.75	108.53	82.64	116.31	153.04	75.80	112 ± 12
61	76.63	43.24	74.38	77.26	77.57	45.29	67.02	91.14	56.17	61 ± 2
62	46.86	34.43	45.44	45.75	55.57	30.37	38.95	55.20	42.87	39 ± 6
64	18.36	28.28	17.77	16.15	28.74	11.89	13.49	21.23	27.04	5 ± 1

Table 4.6: The cross-sections for the (n, α) reaction on Ni isotopes calculated by utilizing the systematic formulas provided in the Table 4.2.

A	$\sigma_{(\mathrm{n},\alpha)}$ (mb) around 14.5 MeV								
	Levkovski	Forrest	Ait-Tahar	Kasugai et al.	Konobeye et al.	Csikai et al.	Habbani et al.	Hingu et al.	EXFOR data
58	133.62	71.53	138.05	97.36	98.36	141.53	131.44	211.55	125 ± 15
62	19.75	21.93	19.29	20.95	21.58	23.50	26.40	23.64	23 ± 2
64	8.31	13.24	7.91	10.45	6.49	9.76	12.76	8.77	11 ± 0

Table 4.7: The cross-sections for the $(\mathrm{n}, 2\mathrm{n})$ reaction on Ni isotopes calculated by utilizing the systematic formulas provided in the Table 4.3.

A	$\sigma_{(\mathrm{n,2n})}$ (mb) around 14.5 MeV						
	Chatterjee et al.	Lu and Fink	Bychkov et al.	Habbani et al.	J. Luo	Hingu et al.	EXFOR data
58	789.87	426.97	454.99	600.01	22.81	112.31	24.70 ± 1.68
61	879.75	769.20	758.27	763.93	389.56	599.56	No data

4.5 Conclusions

In this study, three new systematic semi-empirical formulas were developed from literature data available in the EXFOR library to evaluate $(\mathrm{n, p})$, (n, α), and $(\mathrm{n, 2n})$ reaction cross-section data at the neutron energy of 14.5 MeV. The predicted cross-sections obtained from the formulas demonstrated strong consistency with the literature data. The $\mathrm{F/n}$ ratio for the current formulas exhibits a significant improvement compared to the earlier formulas. The relative error for the present formulas shows an excellent accuracy of the prediction over the considered mass range of nuclei. The developed systematic formulas are useful for a more accurate prediction of neutron-induced reaction cross-sections at 14.5 MeV for different target nuclei within the mass regions $24 \leq \mathrm{A} \leq 238$ for (n, p) reaction, $26 \leq \mathrm{A} \leq 181$ for (n, α) reaction, and $45 \leq \mathrm{A} \leq 238$ for (n, 2n) reaction, respectively.

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