Modeling Excitation Functions for Cobalt-57 Production Using natural Iron-Nickel-Copper Targets for Medical Applications

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Abstract: Nuclear medicine plays a vital role in modern healthcare, utilising radioisotopes for various purposes. Approximately 95% of these radioisotopes are used for diagnostic imaging, while the remaining 5% contribute to treatment applications. Cobalt-57 radioisotopes are used in medical practise for diagnostics and radiotherapy. The excitation functionsns to produce 57Co radioisotope for medical applications using natural iron (Fe), nickel (Ni),i) and copper (Cu) for the reactions natFe(a,x)57Co, natFe(d,x)57Co, natFe(p,x)57Co, natNi(n,x)57Co, natNi(d,x)57Co, natNi(p,x)57Co, natCu(d,x)57Co, natCu(g,2n) 57Co are performed theoretically by Monte Carlo calculations with the TALYS 1.6 nuclear reaction simulation code. Theoretical calculated results are compared with available experimental data in the EXFORlibrary.

***Keywords*:** TALYS 1.6 code; ^{57}Co radioisotope, Exitation functions; Medical isotope production.

1. Introduction

In the field of nuclear medicine, radioisotopes are used for various diagnostic and therapeutic purposes. Approximately 95% of the radioisotopes are used for diagnosis and 5% for treatment. The radioisotopes utilised in nuclear medicine can be administered to the body, allowing for the acquisition of three-dimensional images of the corresponding organ and cells. The production of radioisotopes is essential. In order to manufacture radiopharmaceuticals, the radioisotopes must possess specific physical and chemical properties. Typically, the process for producing radioisotopes involves certain established methods. Usually for radioisotope production by 1. Radioisotope production in reactor system. 2. Radioisotope production in accelerator systems 3. Radioisotope production is used in generator systems. One of the biggest problems in the field of nuclear physics is experimental cost. In this case, the experimental must be high yield. Comparison of theoretical calculations with experimental data is an important contribution to the development of theoretical studies. The properties of the nuclide 57Co make it interesting as a brachytherapy source. The half-life of 57Co

is long (271.79 days), which limits its use in a broad range of clinical diagnostics. 57Co emits photons at 136 keV and 122 keV and decays to stable 57Fe by an electron capture mechanism, as shown in Figure 1 [1]. The factors that determine the usefulness of a radionuclide complex as a tumor-localizing agent include the biological stability of the complex and the uptake and clearance of radioactivity in different organs and tissues.57Co is employed as a radiolabel for vitamin B12 in Schilling's test, which is a diagnostic test studying the gastrointestinal absorption of vitamin B12. The Schilling test was one of the earliest nuclear medicine laboratory services, and it still remains a very useful test in the investigation and management of megaloblastic anemia, as well as malabsorption caused by gastrointestinal disorders.is also employed as a marker in the estimation of organ size and in in-vitro diagnostic kits andical gamma cameras plays a role in the production of calibration standards and sources for radiometric equipment. Recently, 57Co-labeled bleomycinmonstrated greater sensitivity compared to 67Ga in detecting certain tumors. While patients with good renal function experience a low absorbed dose, the widespread use of this radionuclide has been limited due to contamination risks associated with its 270-day half-life. Unlike 67Ga, 57Co Bleomycin is processed by the kidneys without accumulating in normal tissues [2].

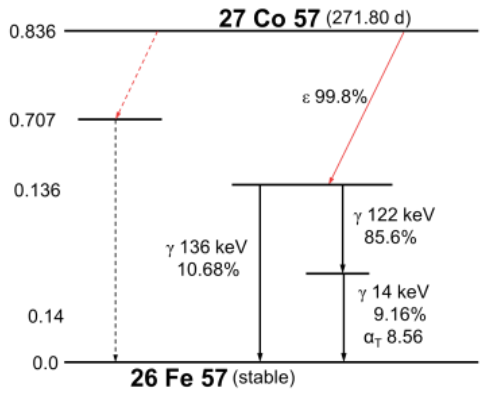

Fig. (1): Cobalt-57 decay scheme [1]

2. Materıal and Methods

In modern medical practices, nuclear medicine plays a significant role in the diagnosis and treatment of many diseases. It comprises a wide range of applications involving medical imaging, tumor assessment, nuclear imaging in case of primary malignancies of the bone, cancers, and so on with various radioisotopes. To generate radioisotopes nuclear reactions are required to produce radioisotopes. The cross section is useful for estimating the probability of nuclear reactions.

There are several ways to get a cross section of the nuclear reaction. The most common one among them is the cross-sectional measurements obtained by experimental methods. The other method-for the calculation of cross-section is obtained by theoretical calculations, which are achieved by the nuclear models. Reactional cross-section calculations obtained by the experimental methods are composed of

various studies in the world and these studies are appended online in the database[3].

There are four radioactive isotopes of cobalt ^{56}Co, ^{57}Co, ^{58}Co and ^{60}Co are human made. also ^{59}Co isotope found in nature but it not radioactive and exists in soil, rocks, water, humans, plants. Radioisotopes of Co are widely used in nuclear medicine, especially ^{60}Co where 70% of cancer patients requiring treatment receiving radiation from this isotope. Table 1 shown the properties of natural and industrial main isotopes of ^{27}Co [4]. Each term in the table means Natural Abundanc is the percentage of a specific isotope found in a naturally occurring element. ^{59}Co is the only stable isotope, making it the sole contributor to natural Co. Half-Life define as the time it takes for half of a radioactive isotope's nuclei to decay. The shorter half-life, the more unstable isotope.

Electron capture (EC) refers to the radioactive decay process in which core electrons are captured by the nucleus, converting protons to neutrons and emitting neutrinos. Betadecay (β-) refers to a radioactive decay process in which neutrons in the nucleus decay in to protons, electrons (beta-particles), and anti neutrinos. Gamma ray emission (γ-) is the emission of high-energy photons from the excited nucleus during radioactive decay. The isotopic properties of cobaltare shown in Table 1.

Table 1: Properties of main isotopes of Co.

Nuclide	Atomic mass	Natural abundance	Half life	Mode of decay	Nuclear spin
^{56}Co	55.940	0 %	77.27 days	EC	4
^{57}Co	56.936	0 %	271.79 days	EC	7/2
^{58}Co	57.936	0 %	70.86 days	EC	2
^{59}Co	58.933	100 %	stable	____	7/2
^{60}Co	59.934	0 %	5.271 years	β^-, γ	5

The present study involves theoretical calculation of excitation functions of natural isotopes for iron (Fe), nickel (Ni), and copper (Cu) target nuclei in some nuclear reactions. Theoretical calculations have been done using the Monte Carlo simulation-based TALYS 1.6 nuclear reaction programme with suitable input parameters. Experimental data required for comparisonhave been extracted from the IAEAEXFOR database [5].TALYS 1.6 simulates and predicts the outcome of nuclear reactions for neutrons, photons, protons, deuterons, tritons, Helium-3 (^{3}He) and alpha particles for target nuclei with masses of 12 or higher in the energy range from 1 keV to 200 MeV. The total reaction cross-section is calculated and divided into various reaction channels and mechanisms by their respective branching ratios. The code is written in FORTRAN and runs on Linux systems.

3. Results and Discussion

This study investigated the Excitation Functions for producing the radioisotope ^{57}Co through various nuclear reactions

using natural iron (Fe), nickel (Ni), and copper (Cu) target nuclei for the nuclear reactions $^{nat}Fe(a,x)^{57}Co$, $^{nat}Fe(d,x)^{57}Co$, $^{nat}Fe(p,x)^{57}Co$,$^{nat}Ni(n,x)^{57}Co$,$^{nat}Ni(d,x)^{57}Co$, $^{nat}Ni(p,x)^{57}Co$,$^{nat}Cu(d,x)^{57}Co$,$^{nat}Cu(g,2n)^{57}$ Co. The calculations employed the TALYS 1.6 simulation code and were compared with existing experimental data from EXFOR database. This study presents the key findings and discusses potential reasons behind the observed agreement or discrepancies between the calculated and experimental results for each reaction (Figures 2-9).

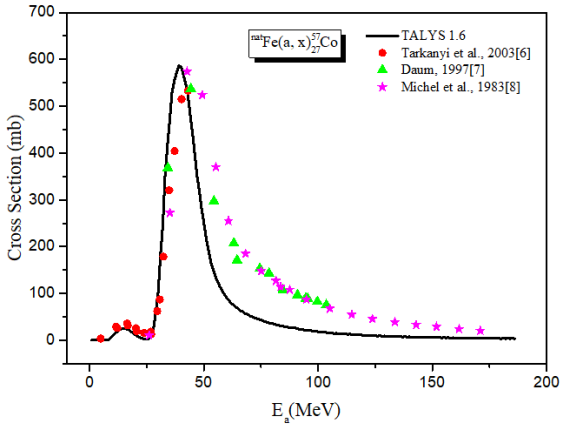

Fig. (2): The comparetion of calculated cross-section of $^{nat}Fe(a,x)^{57}Co$ reaction with experimental data.

Graph in Fig. (2, for the $^{nat}Fe(a,x)^{57}Co$ reaction reveals a distinctive double-peaked structure. The first peak, attributed to the $^{54}Fe(a,n)$ reaction, occurs at 18 MeV and extends to 25 MeV. The second peak at 45 MeV results from combined contributions of ^{54}Fe (a,n) and $^{55}Fe(a,2n)$ reactions, appearing at energies above 25 MeV. The calculated excitation function exhibits excellent agreement with published data, particularly in the low-energy region up to 45 MeV, after this energy the calculated excitation function exceeds experimental data. The primary peak reaches approximately 20 (milli barn) mb, while the secondary peak achieves about 600 mb.

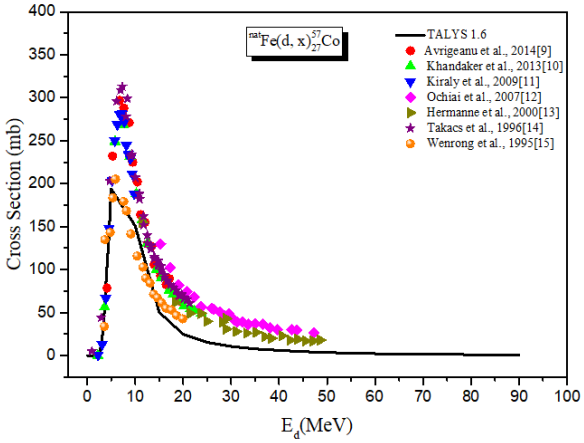

Fig. (3): The comparetion of calculated cross-section of $^{nat}Fe(d,x)^{57}Co$ reaction with experimental data.

Figure 3 shows the calculated excitation function of producing the isotope 57Co when bombarding natural iron with deuterons (d) in the natFe(d,x)57Co reaction compared with existing experimental measurements from the EXFOR database. The calculated excitation function significantly underestimates the experimental data throughout the energy range except at the low energy match;tions perfectly match. This suggests current models might not fully capture complexities of deuteron reactions, like breakup into separate proton and neutron interactions

introducing additional reaction pathways.

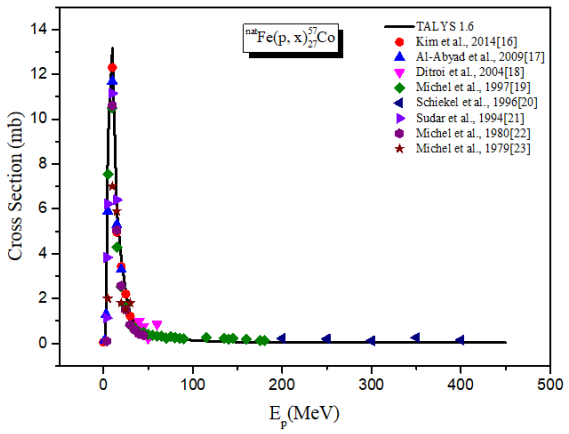

Fig. (4): The comparetion of calculated cross-section of $^{nat}Fe(p,x)^{57}Co$ reaction with experimental data**.**

In Figure 4 the calculated excitation function exhibits a better agreement with the experimental data compared to the previous figures (Figures 2 and 3). This suggests that the theoretical model might be more accurate for proton-induced reactions on natural iron (natFe) compared to reactions with alpha particles (Figure 2) or deuterons (Figure 3).Protons are simpler projectiles than alpha particles or deuterons, and the model might account for their interactions with the target nucleus more effectively. Interestingly, the calculated curve significantly agrees with the experimental values across the entire energy range displayed (0 to 400 MeV).

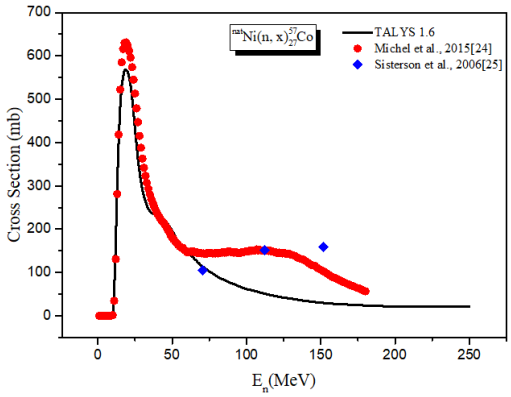

Fig. (5): The comparetion of calculated cross-section of $^{nat}Ni(n,x)^{57}Co$ reaction with experimental data.

The graph in Fig. (5 depicts the calculated excitation function of the $^{nat}Ni(n,x)^{57}Co$ reaction plotted against experimental data. The excitation function signifies the probability of this neutron-induced reaction occurring at various neutron beam energies, leading to the formation of the isotope ^{57}Co in the target ^{nat}Ni. As noted our theoretical results demonstrate excellent agreement with experimental data reported by Michel et al (2015) [24] at low energies and in the energies range between 40-60 MeV. At energies higher than 60MeV, we notice an increase in the cross-section, which may be due to the appearance of another peak due to the interference of another reactions, as one of the data points provided by Sisterson et al (2016) [25] supports this prediction.The cross section exhibits a well-defined peak around 20-25 MeV, with experimental values reaching 640 mb while our calculations predict a maximum of about 570 mb.

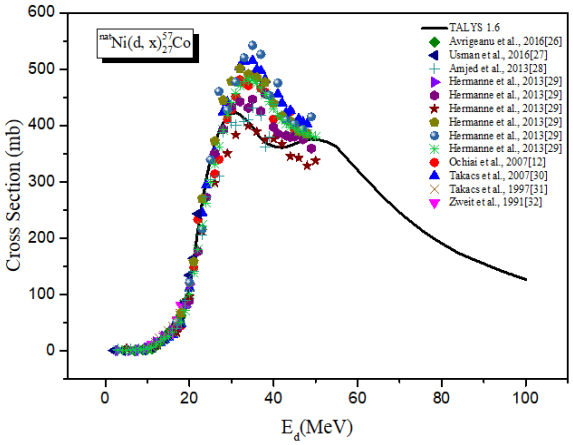

Fig. (6): The comparetion of calculated cross-section of $^{nat}Ni(d,x)^{57}Co$ reaction with experimental data**.**

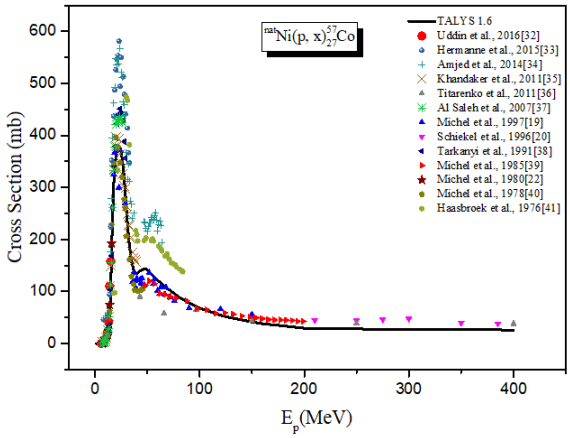

Fig. (7): The comparetion of calculated cross-section of $^{nat}Ni(p,x)^{57}Co$ reaction with experimental data.

Fig. (6 presents a comparetion between theoretical calculations and experimental data for the $^{nat}Ni(d,x)^{57}Co$ reaction. The cross section indicates the probability of this deuteron-induced reaction occurring at various deuteron beam energies. Compatibility is excellent at low energies up to 25 MeV, as for energies higher than 25 the possible reasons for incompatibility it may be caused by model limitations for deuteron reactions compared to simpler projectiles like protons or alpha particles, deuterons have a more complex structure. The $^{nat}Ni(d,x)^{57}Co$ reaction calculations reveal a complex pattern with two distinct peaks. The first peak occurs at 30 MeV, starting at 17 MeV. The second peak apearing at energies above 42 MeV, creating a second peak at 50 MeV, the apearing of the two peak to attributed to combined contributions of another reactions.

The theoretical calculations for the $^{nat}Ni(p,x)^{57}Co$ nuclear reaction demonstrate strong consistency with existing experimental data across an energy range from below 25 MeV and at energy between 26-40 MeV presented in Fig. (7. In the first peak region, experimental data exceed our calculated results by approximately 30%. Conversely, at the second peak which strat apearing at 40 MeV, practical data shows lower values than our calculations except the data presented from Amjed et al (2014) [34] and Haasbroek et al (1976) [41] were shows higher than the calculated results. The cross-section of primary peak between 20-30 MeV reaches approximately, to 600 mb compared to our theoretical prediction of 390 mb.

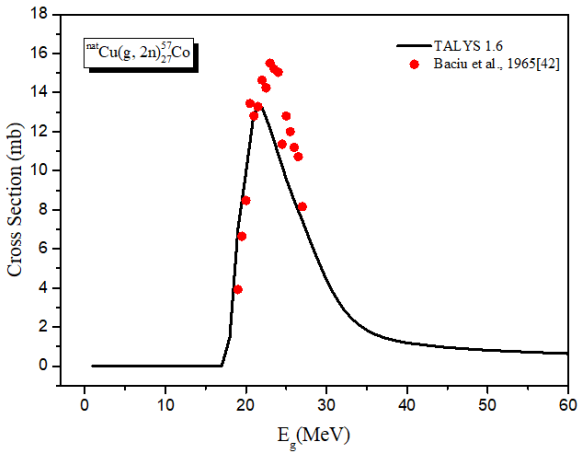

Fig. (8): The comparetion of calculated cross-section of $^{nat}Cu(g,2n)^{57}Co$ reaction with experimental data**.**

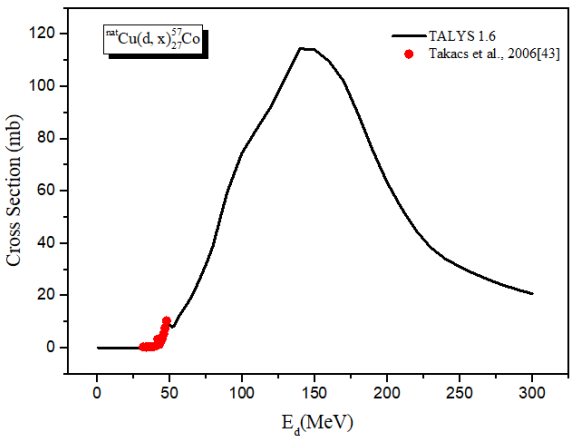

Fig. (9): The comparetion of calculated cross-section of $^{nat}Cu(d,x)^{57}Co$ reaction with experimental data**.**

The $^{nat}Cu(g,2n)^{57}Co$ reaction calculations were compared with the single experimental study from EXFOR library, conducted by Baciu et al. (1965) [42] as in Fig. (8. An excellent agreement is observed up to 22 MeV, though the experimental data shows a 2 MeV shift to the right in the peak region compared to our calculations. The cross-section reaches its maximum around 22-24 MeV, with experimental values approaching 16 mb while our theoretical model predicts approximately 13 mb.

Figure 9 shows excellent agreements in low energies up to 50 MeV conducted by Takacs et al. (2006) [43]. Unfortunately, without access to other experimental data for higher energies, it's difficult to definitively determine if the calculated excitation function agrees with the experimental data. The theoretical model TALYS used in the calculations can predict the reaction probability of natCu(d,x)57Co over the presented energy range. A thorough analysis of these reactions offers significant insights into the mechanisms behind 57Co production. The strong alignment observed between theoretical calculations and experimental data, albeit with some variations in peak regions, confirms the predictive reliability of the TALYS 1.6 code for these reaction pathways. Considering the scarcity of experimental data for certain reactions, especially natCu(g,2n)57Co and natCu(d,x)57Co, the theoretical calculations presented here serve as a

valuable foundation for guiding future experimental studies. Conclusions This study investigated the excitation functions for producing the radioisotope 57Co using various nuclear reactions on natural Fe, Ni, and Cu targets. The analysis revealed both agreements and discrepancies between the calculated results from TALYS 1.6 and the experimental data. The observed discrepancies highlight the limitations of current models in capturing the complexities of reactions involving deuterons and alpha particles. This study has shown a good agreement between the theoretical Excitation Functions results using nuclear reaction simulation TALYS 1.6 code and the experimental data from EXFOR by induced deuterons,tons, neutrons, gamma, alpha particles on Fe, Ni, and Cu target nuclei by different reactions to produce 57Co radioisotope. 57Co is an important medical radioisotope for the diagnosis andy of various diseases used in single photon emission tomography (SPECT). The study emphasisesnce of future research directions, including improved nuclear potential models, advanced computational techniques, integration of nuclear structure data, and the potential of machine learning for further refinement of nuclear reaction modeling. By addressing these limitations and exploring new research directions, scientists can achieve more accurate predictions for isotope production using various nuclear reactions, paving the way for advancements in nuclear medicine, radioisotope production, and fundamental nuclear physics research. Figure 9 showseements in low energies up to 50 MeV conducted by Takacs et al. (2006) [43]. Unfortunately, without access to otherata for higher energies, it's difficult to definitively determine if the calculated excitation function agrees with the experimental data. The theoretical model TALYS used in the calculations can predict the reaction probability of natCu(d,x)57Co over the presented energy range. A thorough analysis of these reactions offers significant insights into the mechanisms behind 57Co production. The strong alignment observed between theoretical calculations and experimental data, albeit with some variations in peak regions, confirms the predictive reliability of the TALYS 1.6 code for these reaction pathways. Considering the scarcity of experimental data for certain reactions, especially natCu(g,2n)57Co and natCu(d,x)57Co, the theoretical calculations presented here serve as a valuable foundation for guiding future experimental studies. Conclusions This study investigated the excitation functions the radioisotope 57Co using various nuclear reactions on natural Fe, Ni, and Cu targets. The analysis revealed both agreements and discrepancies between the calculated results

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