Journal of Science Research and Reviews

PRINT ISSN: 1595-9074
E-ISSN: 1595-8329
DOI: https://doi.org/10.70882/josrar.2024.v1i1.2
Homepage: https://josrar.esrgngr.org

*Original Research Article*

# Optimization of Input Parameters for Enhanced Production of Technetium-99 using the EXIFON Code

***[1]Ibrahim, Nura, [2]Joseph, Emmanuel, [3]Ige, Olumide O., [3]Emmanuel, Adoyi J. and [4]Abdulrazaq, Ahmad**

[1] Nigerian Nuclear Regulatory Authority, North West Zonal Office Katsina, Katsina State, Nigeria
[2]Department of Physics, Federal University Dutsin-Ma, Katsina State, Nigeria
[3]Department of Physics, Nigerian Defence Academy, Kaduna, Kaduna State, Nigeria
[4]Katsina State ICT Directorate Complex, Katsina, Katsina state, Nigeria
*Corresponding Author's email: mfwzee@yahoo.com

**KEYWORDS**
Excitation function,
$^{99m}$Tc,
EXIFON code,
Technetium-99,
ENDF.

**CITATION**
Ibrahim, N., Joseph, E., Ige, O. O., Adoyi Joseph, E. ., & Abdulrazaq, A. (2024). Optimization of Input Parameters for Enhanced Production of Technetium-99 using the EXIFON Code. *Journal of Science Research and Reviews*, *1*(1), 19-23. https://doi.org/10.70882/josrar.2024.v1i1.2

**ABSTRACT**
Radioisotopes are critical in nuclear medicine for both imaging and therapeutic applications. In this work, the optimization of input parameters for enhanced production of technetium-99 using the EXIFON code have been studied. The reaction $^{100}$Mo(p, 2n)$^{99m}$Tc was examined within an incident proton energy range of 0 - 40 MeV. The calculated excitation function for the reaction channel reached a peak value of 1003.7 mbat about 21.00 MeV incident energy. Results obtained from the EXIFON code were compared with evaluated nuclear cross-sections data (ENDF) and experimentally measured cross-sections data (EXFOR) from the International Atomic Energy Agency (IAEA) nuclear database. Our findings show good agreement with the evaluated nuclear data and disagreement with the experimental data within the investigated energy range.

## INTRODUCTION

The production of radioisotopes for nuclear medicine is crucial due to their extensive use in tomography devices and growing applications in various fields (Art & Aytekin, 2015, Joseph et al., 2018). In nuclear medicine, radioisotopes are essential for both diagnostic and therapeutic purposes (Agassi et el., 1975), with their specific properties determining their application. Technetium-99m ($^{99m}$Tc), isolated from molybdenum-99 decay in 1938, is the most commonly used radioactive isotope tracer for SPECT imaging across numerous organs due to its short six-hour half-life, which minimizes radiation exposure (Papagiannopoulou, 2017; Art & Aytekin, 2015; Green, 2012; Adams, 2022). It works by emitting gamma rays detected by a gamma camera (Herman et al., 2007; Uzunov et al., 2018; Joseph & Adams, 2022). Various methods have been employed to analyze the production excitation function of $^{99m}$Tc. Quantum mechanical pre-equilibrium model, the Exifon 2.0, has been adopted for this study to analyze the production excitation function of $^{99m}$Tc in order to obtain the production yield and purity index of the reaction channel of interest. Several models for nuclear reactions exist, and they have the ability to forecast cross sections for these reactions. Among these models are Talys code (Koning, 2012), Empire code (Herman et al., 2007), ALICE code (Agassi et el., 1975), Exifon code and few others. Each of these models has its own strengths and limitations, with some being more powerful than others. The Exifon code is an easy-to-use tool designed for predicting cross sections of nuclear reactions involving uncharged neutrons and gamma rays, as well as charged particles such as protons and alpha particles. Though relatively old (due to the lack of substantial updates in recent years) and lacks the sophistication found in other codes, such as the Talys code, the Exifon code can swiftly estimate the cross sections of nuclear reactions within a few minutes or even a fraction of a minute, depending on the maximum energy of interest. The code holds the advantage of being simple to comprehend and execute, without the need for complicated procedures and substantial effort. Additionally, various prior studies have utilized the code to perform calculations of cross sections (Joseph et al., 2015; Ahmad et al., 2017; Ahmad et al., 2019; Chad-Umoren & Ebiwonjumi, 2014; Dauda, 2011; Joseph & Rabiu, 2013; Dauda, 2017; Jonah, 2004; Hauser & Feshback, 1952; Kalka, 1991; Kalka et al., 1990; Muhammed et al., 2011; Murata, 1997; Polster & Kalka, 1991; Usman & Ahmad, 2020). Moreover, the information from available literature shows that no such work, particularly on excitation function calculation of the production route of $^{99m}$Tc has been carried out; hence, this research is focused on the optimization of input parameters that will enhance the production of technetium-99 using the EXIFON code.

## THEORETICAL FRAME WORK

The EXIFON code is an advanced analytical model that functions within a purely statistical multi-step reaction framework. It provides a comprehensive description of emission spectra, angular distributions, and activation cross sections, encompassing equilibrium, pre-equilibrium, and direct (both collective and non-collective) processes. The model is specifically designed for reactions induced by neutrons, protons, and alpha particles, with these same particles, along with photons, present in the exit channels. Moreover, EXIFON's predictions serves as a valuable complement to experimental data by providing a theoretical basis for understanding nuclear reactions, optimizing production parameters, and enabling efficient planning and execution of experiments for $^{99m}$Tc production.

The quantum mechanical pre-equilibrium model, Exifon 2.0, can be used to analyze the production excitation function of $^{99m}$Tc, focusing on production yield and purity index. Several nuclear reaction models, including Talys, Empire, ALICE, and Exifon, can forecast cross-sections. Exifon is an easy-to-use tool for predicting cross sections for both uncharged and charged particles, though it is relatively outdated compared to more advanced codes like Talys. Despite its simplicity and the lack of recent updates, Exifon is advantageous for its quick calculations and ease of use, requiring minimal effort to operate.

The development of this model was shaped by three pivotal concepts: the classification of nuclear states based on their complexity or exciton numbers as introduced by (Griffin, 1967), the differentiation between bound and unbound states has been outlined (Feshbach, 1980) and the use of random matrices to represent chaotic nuclear Hamiltonians, has been earlier proposed (Agassi et al., 1975). These theoretical ideas were implemented in multi-body theories using the Born series expansion, with residual interactions treated through random matrix theory. This approach enabled the derivation of differential cross-sections for reactions like (a, xb) after energy ensemble averaging as seen in equation (1):

$$(a, xb) = (SMD) + (SMC) + (MPE) \tag{1}$$

where SMD is the statistical multi-step direct process, SMC statistical multi-step compound process and Multi particle emission (MPE) process calculated in a pure SMC concept.

In the statistical multi-step model, the total emission spectrum of the process (a, xb) is divided into three main parts (Kalka, 1991) (see equation 2):

$$\frac{\mathrm{d}\sigma_{\mathrm{a,xb}}(\mathrm{E_a})}{\mathrm{dE_b}} = \frac{\mathrm{d}\sigma^{\mathrm{SMC}}_{\mathrm{a,b}}(\mathrm{E_a})}{\mathrm{E_b}} + \frac{\mathrm{d}\sigma^{\mathrm{MPE}}_{\mathrm{a,xb}}(\mathrm{E_a})}{\mathrm{E_b}} \tag{2}$$

where $\frac{\mathrm{d}\sigma^{\mathrm{SMC}}_{\mathrm{a,b}}(\mathrm{E_a})}{\mathrm{E_b}}$ is SMC emission which is based on a master's equation and $\frac{\mathrm{d}\sigma^{\mathrm{MPE}}_{\mathrm{a,xb}}(\mathrm{E_a})}{\mathrm{E_b}}$ is Multiple Particle Emission Process (MPE), reaction which include the second chance, third chance emission etc. summarized in this term as presented in equation (3):

$$\sum_c \frac{\mathrm{d}\sigma_{\mathrm{a,cxb}}(\mathrm{E_a})}{\mathrm{dE_b}} + \sum_c \frac{\mathrm{d}\sigma_{\mathrm{a,xb}}(\mathrm{E_a})}{\mathrm{dE_b}} \ldots\ldots \tag{3}$$

The first and second term together i.e. (SMC + SMD) represent the first chance emission process. The SMD cross-section is the sum over S-step direct processes given (equation 4) as

$$\frac{d\sigma^{SMD} E_a}{dE_b} = \sum_{s=1} \frac{d\sigma^{(s)}_{a,b}}{dE_b} \tag{4}$$

The Code is based on optical potentials and includes both statistical multistep (SMD) and statistical multistep compound (SMC) components as shown above. EXIFON can perform calculations for incident energies up to 100 MeV quickly and can predict cross-sections using a global parameter set, with outputs formatted in ENDF-6 (Griffin, 1967). The initial step to properly run the program is to ensure that the existing version of EXIFON on the system is functioning efficiently. Typically, the code is installed on a 32-bit operating system. For this study, input parameters were carefully defined, including the use of proton particle as projectile and the $^{100}$Mo isotope of molybdenum as the target nuclei. The code offers a modification option for calculations with or without shell effect corrections; for this study, calculations were performed without shell corrections.

## RESULTS AND DISCUSSION

The energy of the incident proton particle was varied from 0 MeV to 40 MeV, obtaining the cross-section for each energy level. These results were used to determine the excitation function of the reaction. The output data (OUTEXI) used was the energy values to the corresponding cross section data for each reaction. These results are stored in the designated output directory and presented for every possible reaction energy in MeV with their corresponding cross-sections in barns. Other information displayed in the results was discarded because of the objectives of this research work. The calculated cross-section data were then plotted as a function of proton energy, and the resulting excitation curve was compared with Evaluated Nuclear Data (ENDF) from the IAEA nuclear data service website (Kalka, 1991), as well as experimental data from the EXFOR Data Library (Koning, 2012; Lamere et al., 2019).

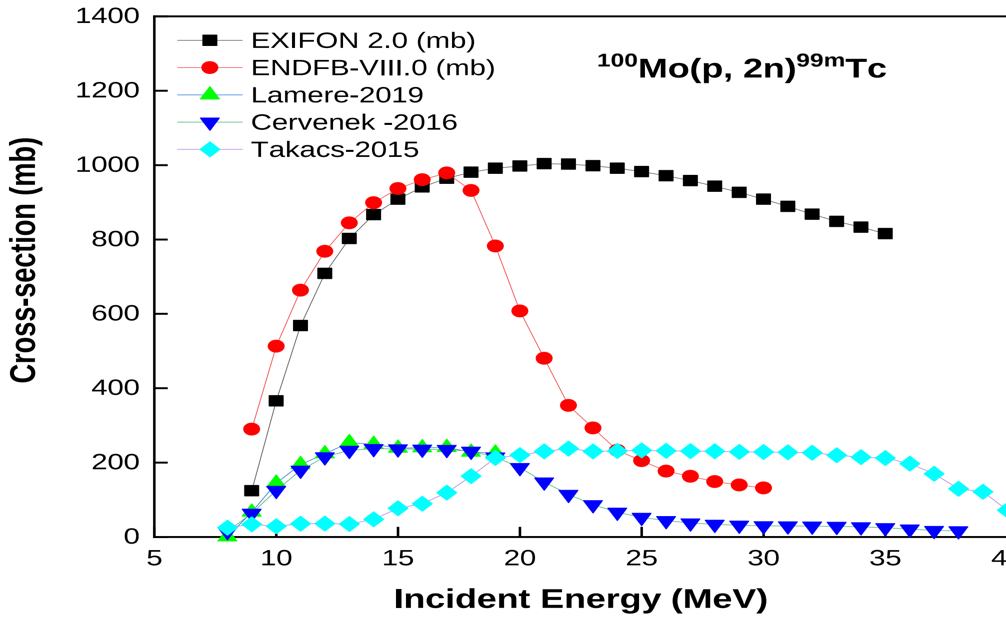


Figure1: Excitation Functions for the $^{100}Mo(p, 2n)^{99m}Tc$ Reaction

The predictions of cross-sections from this study partially align with the ENDF, especially up to about 18 MeV. The EXIFON-estimated cross-sections exceed the ENDF data beyond 18 MeV, up to approximately 30 MeV. Overall, this study predicts higher cross-sections up to around 21 MeV of incident proton energy. As shown in Fig. 1, the detailed shape of the excitation function peaks at about 21 MeV for $^{99m}Tc$ production, with a corresponding cross-section value of 1003.7mb, indicating a region of higher yield production potential. Both EXIFON and ENDF could not accurately replicate the experimental results of (Agassi et al., 1975; Kalka, 1991], despite sharing a similar shape rather than magnitude.

**Table 1: presents the production yield and purity index of the reaction**

| Reactions | Energy of Peak Cross Section ($E_p$) (MeV) | Peak Cross Section Value ($\sigma_p$) (mb) | Total Cross Section ($\sigma_T$) (mb) | Purity Index (PI) (%) |
|---|---|---|---|---|
| $^{100}Mo(p,2n)^{99m}Tc$ | 21.00 | 1003.7 | 23162.8 | 4.33 |

For this work however, the direct dependence of the Yield on the peak cross section has been applied to analyze the yield of the reactions of interest as given in Table 1.

## CONCLUSION

The excitation function for the theoretical production of $^{99m}Tc$, a crucial radionuclide in nuclear medicine, was investigated through proton bombardment of $^{100}Mo$ using the EXIFON nuclear reaction code. The set objective was achieved as the results were compared with experimental data from the EXFOR library and evaluated data for validation and the comparison indicates that the prediction of $^{99m}Tc$ via the investigated method and code is relatively accurate. These findings could aid in providing valuable information for the experimental production of the $^{99mTc}$ radioisotope. In addition, it helps in development and enhancement of future versions of the EXIFON code and other nuclear reaction codes.

## REFERENCES

Adams C, Banks KP, (2023). 'Kubler-Ross stages of dying and subsequent models of grief', in *StatPearls*. Treasure

Island (FL): StatPearls. Available at: http://www.ncbi.nlm.nih.gov/books/NBK430685/ (Accessed: 3 January 2024).

Agassi, D., Weidenmulter, H.A. & Mantzouranis, G. (1975). Generalized Exciton Model for the Description of Preequilibrium Processes. *Phy. Rep*. **22,** 145.

Ahmad I, Yola, Y.I., Koki, F.S. (2017). Evaluation of Excitation Functions of Reactions Used in production of Some Medical Radioisotopes.International Journal of Medical Physics, Clinical Engineering and Radiation Oncology, 6 (3), 290 – 303.

Ahmad I., Fatima Salman Koki, and Yahaya Ibrahim YolaYahaya (2019). Calculation of Reaction Cross-section of Proton-induced Nuclear Reactions on Iodine-127 Isotope. *Bayero Journal of Pure and Applied Sciences* 11(1), 308 – 314.

Art, O. and Aytekin, H (2015). Calculations of Excitation Functions of Proton, Alpha and Deuteron Induced Reactions for Production of Medical Radioisotopes 122 – 125I.Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 345, 1-8.

Chad-Umoren Y. F. and Ebiwonjumi, B. F. (2014). Determination of Nuclear Reaction Cross- sections for Neutron-Induced Reactions in Some Odd – A Nuclides. Advances in Physics Theories and Applications, 32, 55-69.

Dauda A. (2011). Nuclear model calculation of excitation functions of Neutron induced reactions on the structural materials of the miniature neutron source reactor, M.Sc. thesis submitted to the postgraduate school, Ahmadu Bello University, Zaria, Nigeria.

Dauda, A., Jonah, S.A., Hassan, M and Muhammad, B.G. (2017). Nuclear model calculation of excitation functions of neutron induced reactions on the structural materials of the miniature neutron source reactor (Nigeria Research Reactor 1). World Scientific News 66, 86-96.

Feshbach, H., Kerman, A. & Koonin, S. E. (1980). The statistical theory of multi-step compound and direct reactions. *Ann. of Phy*, 125 (2) 429-476.

Green CH. ( 2012). Technetium-99m production issues in the United Kingdom. J Med Phys; 37(2):66-71.

Griffin, J. J. (1967). A Unique Classification of Nuclear States, *Phy. Lett*. **248,** 5.

Hauser, W. and Feshback H. (1952). Inelastic scattering of neutrons, *Physics Rev*. 87, 366 –373.

Herman M., Capote R., Carlson B., Obložinský P., Sin M., Trkov A and Zerkin, V. (2007). EMPIRE: Nuclear Reaction Model Code System for Data Evaluation. *Nuclear Data Sheets* 108 (2007) 2655-2715. https://doi.org/10.1016/j.nds.2007.11.003.

Ige O.O (2009), Nuclear Reaction Cross Section Evaluation from 0 to 20 MeV Using EXIFON2.0 Code, MSC Thesis, Nigerian Defence Academy, Kaduna, February 2009 Calculation of Cross section.

Jonah, S.A. (2018). Nuclear model calculation of excitation functions of neutron induced reactions on the structural materials of the miniature neutron source reactor (Nigeria Research Reactor 1). World Scientific News 66, 86-96.

Jonah S. A. (2004). Shell Structure Effect in Neutron Cross Section Calculation by Theoretical Model Code. *Nigerian Journal of Physics* 16 (2) 81-85.

Kalka H. (1991); Exifon- A Statistical Multistep Reaction Code Report, Technische University Dresden Germany.

Kalka H., Torgman, Lien H. N. Lopezs, Rand Seegler, D. (1990). Description of (n, p) and (n, 2n) Activation Cross Section for Medium Mass Nuclei within Statistical Multi Theory Z. Physics. *Atomic Nuclei,* 335, 163 – 171

Koning, A.J., Rochman, D. (2012). Modern nuclear data evaluation with the TALYS code system. *Nucl. DataSheets*, 113, 2841–2934.

Lamere, M. Couder, M. Beard, A. Simon, A. Simonetti, M. Skulski, G. Seymour, P. Huestis, K. Manukyan, Z. Meisel, L. Morales, M. Moran, S. Moylan, C. Seymour, Stech E. (2019). Proton-induced reactions on molybdenum, University of Notre Dame, Notre Dame, Indiana 46556, USA, DOI: 10.1103/PhysRevC.100.034614.

Muhammed, K., Onimisi, M.Y and Jonah, S.A. (2011). Investigation of the Shell Effect on Neutron Induced Cross Section of Actinides. *Journal of Nuclear & Particle Physics*, 1, 6-9.

Murata, T. (1997). Modification of EXIFON code and analysis of $^{16}$O+n reactions in En=20 50MeV.*JAERI-Conf--97-005,* Fukahori, Tokio (Ed.), Japan.

Papagiannopoulou D (2017). Technetium-99m radiochemistry for pharmaceutical applications. JLabelled CompRadiopharm;60(11):502-520.

Polster, D. and Kalka, H. (1991). Short Note Fission within a Statistical Multistep Model. *ZeitschriftfürPhysika handbook of Hadrons & Nuclei*, 424, 423-424. https://doi.org/10.1007/BF01560648.

Rizk TH, Nagalli S (2023). StatPearls [Internet]. StatPearls Publishing; Treasure Island (FL): Technetium 99m Sestamibi.

Takacs, A., Hermanne, Ditroi, F., Tarkanyi, F and Aikawa M. (2015), Reexamination of cross sections of the 100Mo(p,2n)99mTc reaction, Institute for Nuclear Research, Hungarian Academy of Sciences, 4026 Debrecen, Hungary, Nuclear Instruments and Methods in Physics Research B 347 26–38.

Usman A. R., & Ahmad A. A. (2020). EVALUATION OF $^{67}$Ga CROSS SECTIONS USING EXIFON CODE FOR MEDICAL APPLICATIONS. *FUDMA JOURNAL OF SCIENCES*, *6*(3), 113 - 118. https://doi.org/10.33003/fjs-2022-0603-987.

Uzunov NM, Melendez-Alafort L, Bello M, Cicoria G, Zagni F, De Nardo L, Selva A, Mou L,Rossi-Alvarez C, Pupillo G, Di Domenico G, Uccelli L, Boschi A, Groppi F, Salvini A, Taibi A, Duatti A, Martini P, Pasquali M, Loriggiola M, Marengo M, Strada L, Manenti S, Rosato A, Esposito J (2018). Radioisotopic purity and imaging properties of cyclotron-produced $^{99m}$Tc using direct $^{100}$Mo(p,2n) reaction. Phys Med Biol;63(18):185021.

Joseph, E., Atsue, T. and Adams, S. (2018). Assessment of Radon-222 in Selected Water Sources at Dutsin-Ma Town, Dutsin-Ma Local Government Area, Katsina State, *Journal of Scientific and Engineering Research*, 2018, 5(5):49-59. http://jsaer.com/download/vol-5-iss-5-2018/JSAER2018-05-05-49-59.pdf

Joseph, E., Nasiru, R., Sadiq, U., Ahmed, Y. A. (2015). Energy and Efficiency Calibrations for High Purity Germanium GEM30195 Coaxial Detector USING $k_0$-IAEA Software. *International Journal of Science and Research, Vol. 4, No. 8: 1055 – 1061, India*. *https://www.semanticscholar.org/paper/Energy-and-Efficiency-Calibrations-for-High-Purity-Joseph/daac7ec450f31eb4134a93b3e70c6491ea3205be*

Joseph, E. and Nasiru, R. (2013). Geometry Correction in Efficiency of a Sodium Iodide (Thallium Activated), NaI(Tl) Detector. *Advances in Applied Science Research. 4(1):400-406.* https://www.primescholars.com/articles/geometry-correction-in-efficiency-of-a-sodium-iodide-thallium-activatednaitl-detector.pdf

Adams, S., Joseph, E., & Kamal, G. (2022). Validation of Tritium Calibration Curve in CIEMAT/NIST Activity Measurement Using Non-Linear Least Squared Fittings and Calculations of the Half-Life and Decay Constant of Potassium-40. Journal of the Nigerian Society of Physical Sciences, 4(3). https://doi.org/10.46481/jnsps.2022.621

Joseph, E. and Adams, S. (2022). Determination of Specific Activity of $^{40}$K, Its Half-Life and Decay Constant Using Efficiency Tracing CIEMAT/NIST Method. *Nigerian Journal of Physics*. 31(1), 23 – 31.