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Nuclear Cross Section Evaluation in Particles Induced Reactions on ^{87}Sr and ^{89}Sr for Optimal Production of ^{86}Y And ^{90}Y Radionuclides

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Abstract

The ascend of interest concerning ^{86}Y and ^{90}Y90 radionuclides which lies among the most important radionuclides for therapy of organic tumours has driven up the demand for the radionuclides. The use of enriched Strontium radionuclides for accelerating the production of ^{86}Y via the ^{87}Sr (p,2n) ^{86}Y and ^{90}Y through ^{89}Sr (d,n) ^{90}Y reactions respectively is thus essential in order to generate a wide variety of ^{86}Y and ^{90}Y labelled radiopharmaceutical drugs for treatment benefits of patients. However, these routes, though more plausible than nuclear reactor method, is inundated with a number of competing contaminant radionuclide such as ^{84}Y, ^{85}Y, ^{87}Y and ^{88}Y. In this paper the Q-value and reaction cross sections of the ^{87}Sr (p,2n) ^{86}Y and ^{89}Sr (d,n) ^{90}Y reactions were calculated using GEANT4 toolkit and the effects of Q-Value in optimizing the production of ^{86}Y and ^{90}Y were discussed to evaluate the most favorable nuclear data for optimal production of the nuclides. Q-Value of -14.456 MeV and 5.3451 MeV were found to be most feasible for ^{86}Y and ^{90}Y production respectively along with respective maximum cross sections at incident energy level of 25 MeV and 17.5 MeV. This nuclear data will be very useful for radionuclide production of ^{86}Y and ^{90}Y using accelerators or cyclotrons.

Keywords: *Radionuclide, Radiopharmaceutical, Radiotherapy, Q-Value, Cross Section.*

INTRODUCTION

Theranostics is an emerging paradigm in nuclear medicine that integrates diagnostic imaging and targeted radionuclide therapy into a unified framework. By combining non-invasive imaging, patient-specific dosimetry, and radiopharmaceuticals, this approach allows for individualized treatment planning and precise delivery of therapeutic doses. Such integration not only enhances treatment accuracy but also minimizes toxicity, reduces cost and treatment time, and improves overall clinical outcomes (Rosch *et al.*, 2017; Watabe *et al.*, 2025). The success of theranostics relies on radionuclides that meet strict physical, chemical, and biological requirements. Ideal diagnostic radionuclides have short half-lives (2 -24 h) and favorable positron (β^+) emission for Positron Emission Tomography (PET) or gamma emission for Single Photon Emission Computed Tomography (SPECT). While therapeutic radionuclides typically exhibit longer half-lives (2 -10 d) and emit alpha, beta (β^-) particles or Auger electrons suitable for targeted therapy (Rosch *et al.*, 2017;Loveless *et al.*, 2020). Only a limited number of pairs, such as ^{86}Y/^{90}Y and ^{68}Ga/^{177}Lu, fulfill these requirements, yet their production remains technically demanding and costly (Zubaida & Ahmad, 2024).

However, the growth of interest in ^{86}Y that has a 14.7 hours half-life and ^{90}Y with half-life of 2.67 days was due to successful treatment of patients with certain cancers of the thyroid. The emission characteristics of ^{86}Y and ^{90}Y which include β^+ and gamma emission of 155 KeV respectively makes the radionuclides ideal for combination with vector molecules for theranostic treatment. The accelerator production of Y86 is via a number of reactions including ^{86}Sr(p,n)^{86}Y, ^{86}Sr(d,2n)^{86}Y, ^{88}Sr(p,3n)^{86}Y, ^{nat}Rb(^{3}He,xn)^{86}Y, ^{90}Zr(p,αn)^{86}Y and ^{nat}Zr(p,x)^{86}Y reactions (Choinski & Lyczko, 2021) though many other routes exist but with very small cross sections. Y90 on the other hand is produced mainly via the irradiation of natural Yttrium with thermal neutrons in nuclear reactor by (n,ϒ) reaction. The other way, which most practiced is the use of ^{90}Sr generator in from Uranium fission, equilibrium mixture with ^{90}Y. Nevertheless, in order to promote and widen the use of the radionuclides for radiotherapy and radio diagnostic applications, the use of accelerator has been studied using proton, deuteron and electron beams and the results indicate that the ^{89}Sr89(d,n) ^{90}Y reaction has the biggest cross section at energy of 17.5 MeV, while the reaction Sr87(p,2n) is most feasible for Y86 production, suffice to say low energy production is among

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the prerequisites of theranostic radionuclides (Turler, 2019). The use of natural Sr was also shunned due to impurities of competing radionuclides of Sr which are chemically inseparable and the fact that enriched Sr (Sr87 and Sr 89) has least amount of impurities. The Q-value, which is the net energy change in a reaction is a very important factor and plays a big role in determining reaction feasibility (). Several studies were conducted to assess the Qvalue effects in syntheses of radionuclides such as Jurbandam L (2018) who investigated fission Q-values and energy deposition profiles of Safari I reactor and Graeger (2010) in a thesis that evaluated the effects of Q-value in production of super heavy elements. In spite of the foregoing, incisive studies into the influence of Q-value in reaction probabilities, optimization of reaction products yield and even determination of specific activity is quite condoned in recent times. Thus need exists to look into nuclear reaction energetic as a means of augmenting the mechanisms of production of new radionuclides for the betterment of health of humanity (Uddin *et al.*, 2023). ^{90}Y portrays a wholesome example of diagnostic and therapeutic properties and, as true theranostic, is accessible in the same element. It had a half-life of 2.7 days which suffices the critical dosage levels of radiotherapy. It emits a hefty amount of β- (2.27 MeV) and a little β+ and Υ emission capable of penetration in tissues up to 11mm. The high energy β-emission of Y90 reaches not only the target disease but also swiftly pervades the surrounding tissues with about 90% of the radiation being absorbed in a path length of 5mm. Y86 on the other hand is a predominant β+ emitter with a half-life of 14.7 hours and is useful in theranostics as the agent of diagnostic (PET) imaging while the former undertakes the therapeutic action.

A persistent challenge however, is the lack of reliable low-energy nuclear data, which are essential for optimizing accelerator-based radionuclide production (Usman & Ahmad, 2022). One of such important parameters is the cross section which is the probability of inducing a nuclear reaction and is dependent upon incident particle energy (Shahid *et al.*, 2017). Consequent upon this, the magnitude of cross section can be plotted as particle energy function to generate an excitation function which can be used to determine the optimal particle energies for maximizing the product of the nuclear reaction (Martin, 2006). Without such data, the development of sustainable and scalable production strategies remains limited, especially for novel theranostic candidates.

To address this gap, systematic studies of particle-induced nuclear reactions at medical accelerator energies (≤ 25 MeV) are required. This work investigates the excitation functions for (p,2n) and (d,n) reactions on ^{87}Sr and ^{89}Sr targets for the production of theranostics radionuclide ^{86}Y and ^{90}Y using the GEometry ANd Tracking (GEANT4) simulation toolkit. The objective was to generate precise nuclear data and validate using evaluated and experimental datasets. In doing so, this study aims to contribute to the reliable accelerator-based supply of high-purity theranostic radionuclides, thereby supporting the integration of diagnosis and therapy in modern nuclear medicine.

THEORETICAL BACKGROUND

The production of Y86 and Y90 through proton and deuteron induced reactions respectively on Strontium 87 and Strontium 89 were simulated using GEANT4. The Cross sections and models form the second level of the multilayer framework and are crucial concepts in the simulation. Cross sections determine the location and timing of specific interactions, while models dictate the outcomes of these interactions through calculations, meanwhile considered as the generator of the final state. To calculate reaction cross sections across a broad energy spectrum, the GEANT4 toolkit incorporates the formulas developed by Tripathi, Kox, Sihver, and Shen(Cao *et al.*, 2009). These formulas are parameterized to account for theoretical aspects such as Coulomb corrections, asymmetric proton and neutron numbers, Pauli blocking, and other factors (Folger *et al.*, 2003). This parameterization can be generally expressed as

$$\sigma_R = \pi r_0^2 \left(A_p^{\frac{1}{3}} + A_T^{\frac{1}{3}} + \delta \right)^2 \left(1 - \frac{Bc}{E_{cm}} \right) \qquad (1)$$

Where r_0 is the reduced nuclear radius parameter and is energy independent, A_p and A_T are the mass numbers of projectile and target respectively and E_{cm} is the colliding system centre of mass energy in MeV, δ is either energy dependent or independent parameter. while the last term of the equation is the Coulomb interaction term (with Coulomb barrier Bc) (Rehman *et al.*, 2011). Due to a very short range of nuclear forces, a nuclear reactions can only occur when the incident charged particle is actually incorporated into the target nucleus and when the incident particle and the target nucleus are all positively charged, a large coulomb barrier of repulsion arises which must be overcome. Energy change due to mass transformation during nuclear reaction process is a characteristic that accompany every reaction (Avrigeanu et al., 2012). The net change of this energy in a nuclear reaction is called Q-Value. The Q-value is defined as,

$$Q = \{(m_t + m_p) - (m_r + m_e)\}c^2 \qquad (2)$$

where m_t is the mass of the target, m_p is mass of projectile, m_r; mass of product nuclei, m_e is the mass of ejectile and c is the velocity of light (). We can deduce from above that, if Q >0, $(m_t + m_p) > (m_r + m_e)$ and the reaction is known as exothermic and in this case binding energy or nuclear mass energy is released as the kinetic energy of the final product. However, if Q < 0, $(m_t + m_p) < (m_r + m_e)$ the reaction is said to be endothermic. The initial kinetic energy is absorbed or converted to mass or binding energy, and if Q = 0 elastic scattering occurs, and

$$(m_t + m_p) = (m_r + m_e) \qquad (3)$$

The benefits of determination and understanding Q value are numerous, the former determines the maximal possible kinetic energy of products of nuclear reactions while the latter guides in selection of nuclear reactions for medical radionuclides production. In addition, Q value also influence product yield and potential contaminants and in optimizing production of diagnostic and therapeutic radionuclides it also plays a critical role. Further, from the reaction feasibility perspective, Q Value plays a decisive role as positive Q value reactions can occur spontaneously or with minimal activation energy while negative Q value indicates that reaction require external energy input to proceed because of higher activation energies characterized by endothermic reactions. Q value determination is significant in several nuclear physics applications such as nuclear reactor operations and management, medical isotope production both in reactor based and using cyclotrons, design and implementation of nuclear experiments, astrophysics and many more.

The second crucial concept in this simulation are the models, models determined the outcomes of these interactions through calculations. The intranuclear cascade model simulates the initial stages of nuclear reactions, where incident particles interact with nucleons in the target nucleus. The Bertini cascade model applies to intermediate energy ranges, simulating secondary particle production due to nucleon interactions. The Precompound model describes the formation of an excited nucleus prior to compound nucleus (CN) formation, essential for predicting decay and particle emissions. The evaporation model handles de-excitation of nuclei, simulating particle emission and final states, which are crucial for modelling radioisotope production.

METHOD

GEANT4 is a computational toolkit based on Monte Carlo that simulates the passage of particles through matter. The use of this toolkit is wide across various areas of physics such as medical, astrophysics and high energy. The toolkit is ideal for simulation of irradiations for production of isotopes because it has the ability to model even geometries that are deemed complex and comprises of a large array of theoretical and data driven models. The geometry used is a simple 10cm thick target size that receives particle beam through a foiled tube. The investigation in this paper involves irradiation of enriched Strontium 87 and Strontium 89 targets using proton and deuteron particles respectively for energies up to 25 MeV. The first step in the simulation is the selection of an appropriate physics list. The Intranuclear cascade model, along with Bertini cascade, Precompound and Evaporation models were used for this simulation. Intranuclear model simulates the initial stages of the reactions, Bertini cascade simulates the intermediate energy stage involving the emission of secondaries particles while Precompound model simulates the excite state of nuclear reaction before the Compound Nucleus formation. Evaporation model handles CN de-excitation up to final state via the emission of particles and formation of radioisotopes. Incorporating these models enable simulation of a wide range of nuclear reactions for radioisotope production and emission of particles.

The particle generation phase involves specifying the type of particles and their energies. This is typically done using the GEANT4 particle generator, where a monoenergetic particle beam is defined, and the energy distribution is set based on the deuteron energies from 0 MeV to 25 MeV. The particle-nucleus interactions are then simulated using the selected physics models. Particle interactions with Yb176 are tracked and the reactions such as nuclear excitation and emission of secondary particles are computed. The cross-sections for these interactions are calculated based on the physical models chosen. The nuclear reaction cross-sections for particle-induced reactions are taken from dedicated nuclear reaction models implemented in GEANT4, which account for low-energy reactions. After the interactions data are generated, particles track and energy deposition information are collected. The energy deposited by the deuteron particle and secondary particles (including neutrons, gamma and electrons) in the target nucleus are recorded and used to determine quantities

Uncertainty is typically reported using standard deviation or confidence intervals. For example, for each simulation run, the mean free path and cross-section data are averaged over multiple iterations, and their uncertainties are calculated based on the spread of values observed in different simulation trials. This ensures that the data accounts for statistical fluctuations is handled using standard methods for statistical analysis of the simulation results, which ensures that any uncertainties in the model parameters or particle generation are properly accounted for in the final results. Once the simulation is completed, the results are compared with available nuclear physics data for validation. Corresponding Q-values for the reactions were analyzed to establish correlation with cross section so as to generate the optimal energy for maximum production of isotopes and avoid contamination from competing reaction channels.

RESULTS AND DISCUSSION

The results of simulation of Sr87 (p, 2n) Y86 and Sr89 (d, n) Y90 reactions are presented below; Table 1 shows the corresponding Q values for the reactions.

Table 1. Energy dependent Q values of Sr87 (p, 2n) Y86 and Sr89 (d, n) Y90 reactions

Incident Energy (MeV)	Sr87(p,2n)Y86 (Qvalue) (MeV)	Sr89(d,n)Y90 (Qvalue) (MeV)
1	0	0
2	0	0

3	0	0
4	0	5.4351
5	0	5.4351
6	0	5.4351
7	0	5.4351
8	0	5.4351
9	0	5.4351
10	0	5.4351
11	0	5.4351
12	0	5.4351
13	0	5.4351
14	0	5.4351
15	0	5.3423
16	-14.473	5.3451
17	-14.459	5.3434
18	-14.458	5.3451
19	-14.458	5.3451
20	-14.458	5.3451
21	-14.456	5.3451
22	-14.456	5.3451
23	-14.456	5.3451
24	-14.6	5.3436
25	-14.456	5.3451

For any nuclear reaction route that is aimed to produce a medical radionuclide of choice, the role of Q value is indispensable due to its significant effect on reaction kinetics through altering activation energies of the reaction. Higher Q values leads to lower activation energy barrier thus facilitating faster reaction rates due to increased likelihood of collision, (implying higher cross sections) among reactants. Consequently, higher Q values lead to higher cross sections. Thus as Table 1 indicates positive Q values for the entire energy range of the Sr87 (p, 2n) Y86 and Sr89 (d, n) reactions hence the deuteron induced reaction has higher likelihood and will lead to higher yields. In addition, while Q value for the reactions undergoes little change across the reaction energies, it indicates only interactions and reaction cross sections will play decisive role in optimizing the production of Y86 and Y90. Y90 production however, will be more realistic and will lead to energetic particles since the Sr89 (d,n) reaction is exothermic and hence more energetically favourable when compared to Sr87(p,2n) reaction which, being endothermic will rely on energy absorption from incident protons to proceed and will therefore result in production of low energy particles.

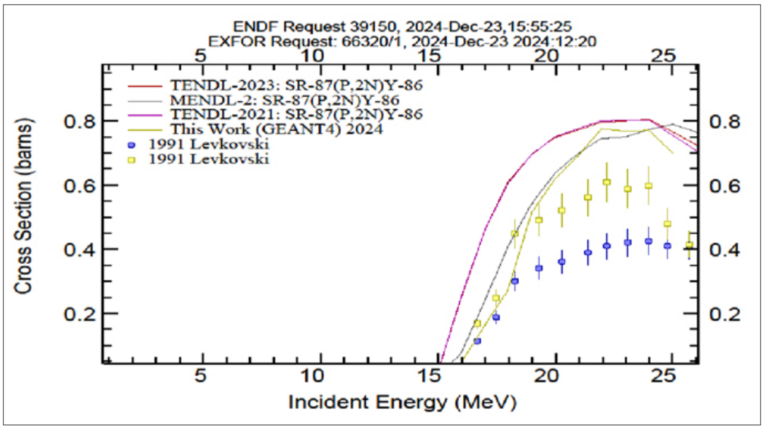

Figure 1. Excitation function of Sr-87(p, 2n) Y-86 reaction

In Figure 1 the excitation function of the reaction Sr-87(p,2n) Y-86 calculated using GEANT4 simulation appears to show remarkable agreement with TENDL- 2023, MENDL -2 and TENDL – 2021 datasets. Both TENDL 2021 and 2023 show slightly higher values with cross sections showing decrease at 24 MeV energy region. The experimental data reported by Levkovski (1991) show lower values than calculated data but on the whole there is good agreement.

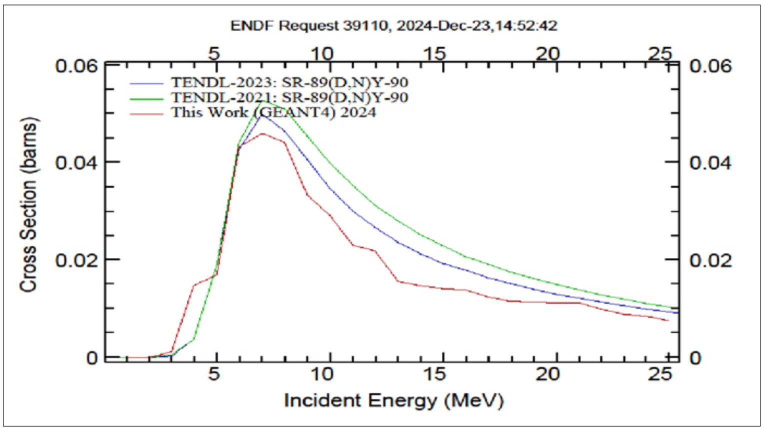

Figure 2. Excitation function of Sr-89(d,n) Y-90 reaction

The figure 2 shows excitation function for Y-90 production using Sr-89(d,n) reaction which indicates undulating values at lower energies and reaches peak cross section at slightly above 0.4 b. While the figure shows good agreement with both TENDL 2021 and 2023 datasets, the latter show higher cross section values while the reaction exhibits possible compound nucleus formation at 8 – 10 MeV region with possible de-excitation afterwards from 13 – 25 MeV.

CONCLUSION

This study as aimed, investigated the production of Y86 and Y90 through proton and deuteron reactions respectively with two different Strontium isotopes with the aim of elucidating the conditions for optimal production of the radionuclides. Y86 is one of the most important therapeutic radionuclides currently employed in theranostic applications for treatment of cancers and bone pain. Y90 is the first radionuclide to be used for theranostic application in treatment of breast cancer. Y90 has a half-life of 2.67 days and decays by emission of large quantities of β- (2.27 MeV) and small amounts of a β+ and ϒ which is penetrative up to 11 mm in tissues. This radionuclide is one of the most important theranostics having both diagnostic and therapeutic properties accessible in one element. Y90's lengthy half-life allows it to achieve critical dosage requirement necessary for radiotherapy and its thus ideal for solid tumors due to its penetrability. Y86, with half-life of 14.7 hours, decays through positron emission and this makes it a promising candidate for pre-treatment dosimetry and PET imaging. Y90 and Y86 together makes matched theranostic pair with outstanding potential for personalized medicine applications.

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