Production of $^{44}\text{Ti} \rightarrow ^{44}\text{Sc}$ Generator in Comparison with Direct Routes by Cyclotrons: Cross Section Evaluation Using Nuclear Models Codes

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ABSTRACT

This paper we presents a comparative study of several nuclear reactions that are used for production of the medical interested radionuclide $^{44}\text{Sc}$. The study includes cross section calculations using TALYS and EMPIRE codes for the nuclear processes that lead to producing the $^{44}\text{Ti}/^{44}\text{Sc}$ generator system on the cyclotron as indirect method for production. The cross section values of the nuclear reactions $^{45}\text{Sc}(p,2n)^{44}\text{Ti} \rightarrow ^{44}\text{Sc}$, $^{45}\text{Sc}(p,n)^{46}\text{Ti}$, $^{45}\text{Sc}(d,3n)^{44}\text{Ti} \rightarrow ^{44}\text{Sc}$, $^{45}\text{Sc}(d,2n)^{46}\text{Ti}$, $^{44}\text{Ca}(\alpha,4n)^{44}\text{Ti} \rightarrow ^{44}\text{Sc}$, $^{43}\text{Ca}(\alpha,2n)^{44}\text{Ti}$ and $^{43}\text{Ca}(\alpha,3n)^{44}\text{Ti} \rightarrow ^{44}\text{Sc}$ were calculated from the threshold energy up to 50 MeV. The obtained theoretical data were compared with the previously reported experimental values and a systematic analysis of the excitation function was done to calculate the radioactive yields of the produced radionuclides. Furthermore, the direct production routes were studied for the proton, deuteron and $\alpha$-particles induced reactions on $^{40,42,43,44}\text{Ca}$ enriched targets for production of the $^{44}\text{Sc}$ radioisotope. The results revealed that a relatively high radioactive yield can be obtained from the direct processes because of the short half-life of $^{44}\text{Sc}$. The generator method is preferred whenever long transport time is needed. The discussion includes factors affecting the elution of $^{44}\text{Sc}$ from its parent nucleus $^{44}\text{Ti}$ that formed in the irradiated target and the theoretical aspects behind the practical application.

Keywords: $^{44m}\text{Sc}$ Radionuclide; $^{44}\text{Ti}/^{44}\text{Sc}$ Generator; Excitation Function; Nuclear Models Code; Statistical Parameter

1. INTRODUCTION

The radionuclide $^{44}\text{Sc}$ with half-life of 3.97h has suitable properties for applications in nuclear medicine as tracer agents for PET imaging. It is a positron emitter with high intensity (94.3%) and suitable energy range for the emitted positrons (1.2-1.5 MeV) (1). The physical characteristics of $^{44}\text{Sc}$ is compared to those of the shorter half-life $^{68}\text{Ga}$ isotope ($T_{1/2} = 67.71$ min) to study long biological processes applying labeled antibodies (2-4). The $^{44}\text{Ti}/^{44}\text{Sc}$ generator is one of the production routes for $^{44}\text{Sc}$ which gained interest by several researchers, but the complicated post-elution purification of the $^{44}\text{Sc}$ limits its applicability (5-10).

Recent intermediate cyclotrons allow direct economic production of $^{44}\text{Sc}$ with adequate yields and radionuclidic purity by p, d or $\alpha$-particle induced reactions on $^{nat}\text{Ca}$ or enriched $^{43,44}\text{Ca}$ (11-17). The isomer $^{44m}\text{Sc}$ ($T_{1/2} = 58$ h) is also of suitable properties that can be employed in nuclear medicine such as using $^{44m}\text{Sc}/^{44}\text{Sc}$ generator for long in-vivo biological study and its relevant labeled antibodies (2,3).
The nuclear reaction cross section data can help to study the possibility of producing $^{44}$Sc radioisotope via direct or indirect routes and evaluate the expected radioactive yield. The reported data for the nuclear reactions $^{40}$Sc(p,2n)$^{42}$Ti→$^{44}$Sc and $^{40}$Ca(p,n)$^{44}$Sc have an indication that there is a high probability for the production of $^{44}$Sc either in low or medium energy range. It is noticed that some inconsistent values of the reported nuclear reactions cross section data for the formation of $^{44}$Sc and therefore theoretical evaluations using nuclear model codes are needed. Furthermore, the lack of the available cross section data that cover d- and α- particle induced reactions result in a significant gap for the predicted radioactive yield and the possible impurity levels.

The purpose of the present study is to evaluate theoretically (using model code calculations) the possible nuclear reaction cross sections for production of $^{44}$Ti→$^{44}$Sc generator with comparison to the available previously reported experimental data. The alternative production routes through direct routes of p, d and α-particles on Ca target were studied for comparison with generator method. The estimated Thick Target Yields (TTY) for all the studied nuclear reactions were evaluated and compared with the experimental values.

### 2. PRELIMINARY NUCLEAR DATA

Nuclear decay data for the target and product radionuclides under investigation in this study are given in scheme(1). Using model code library [1], the $^{44}$Ti decays to $^{44}$Sc by EC mode emitting very low energy γ-rays with energies 67.8 keV ($I_{\gamma}$=93 %) and 78.3 keV ($I_{\gamma}$=96.4 %). The $^{44}$Sc has a long lived isomeric state $^{44}$mSc ($T_{1/2}$ = 58.6 h) decays by IT mode with energy $E_{\gamma}$= 271 keV ($I_{\gamma}$=86.7 %) to the ground state $^{44}$gSc ($T_{1/2}$ =3.9 h). The presence of different isotopes in natural Ca allows the production of different impurities if it is used for direct production routes. These possibilities will be discussed below. The q-values and threshold energies of the nuclear reactions under investigation are given in table(1).

![Table](1): Nuclear chart of the $^{43}$Ti and $^{44}$Sc radioisotopes

<table>
<thead>
<tr>
<th>$^{40}$Sc ($\epsilon+\beta^+$)</th>
<th>$^{41}$Sc ($\epsilon+\beta^+$)</th>
<th>$^{42}$Sc ($\epsilon+\beta^+$)</th>
<th>$^{43}$Sc ($\epsilon+\beta^+$)</th>
<th>$^{44}$Sc ($\epsilon+\beta^+$)</th>
<th>$^{45}$Ti ($\epsilon+\beta^+$)</th>
<th>$^{46}$Ti ($\epsilon+\beta^+$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5909 ms</td>
<td>63 y</td>
<td>58.6 h</td>
<td>3.927 h</td>
<td>100%</td>
<td>8%</td>
<td>100%</td>
</tr>
</tbody>
</table>

| $^{40}$Ca ($69.41\%$) | $^{41}$Ca ($1.03E+5$ y) | $^{42}$Ca ($0.647\%$) | $^{43}$Ca ($0.135\%$) | $^{44}$Ca ($2.086\%$) | $^{45}$Ca ($162.6$ d) | $^{46}$Ca ($0.004\%$) |

Table (1): Nuclear reaction data for the formation of $^{43,44}$Sc and $^{44}$Ti radioisotopes
3. Nuclear models calculation

3.1 TALYS-1.6

We used two computer codes, namely, TALYS-1.6 and EMPIRE-3.2 (Malta)\textsuperscript{(18-20)}, for determination of the investigated nuclear reaction cross sections. The basic construction of TALYS-1.6 is based on pre-equilibrium particle emission approach using the two-component exciton model\textsuperscript{(18,19)}. The computer code EMPIRE-3.2 (Malta) is a modular system of nuclear reaction codes, comprising various nuclear models, and designed for calculations over a broad range of energies and incident particles\textsuperscript{(20)}. The code accounts for the major nuclear reaction models such as optical model, coupled channels and DWBA (ECIS06 and OPTMAN), Multi-step Direct (ORION + TRISTAN), NVWY Multi-step Compound, exciton model (PCROSS), hybrid Monte Carlo simulation (DDHMS), and the full featured Hauser-Feshbach model including width fluctuations and the optical model for fission\textsuperscript{(21,22)}. Comprehensive input parameters are extracted from the RIPL-3 library, which cover the nuclear masses, optical model parameters, ground state deformations, discrete levels and decay schemes, level densities, fission barriers, and γ-ray strength functions.

3. RESULTS AND DISCUSSIONS

3.1 Proton induced reactions

3.1.1 $^{44}$Ca(p,n)$^{44m,g}$Sc, $^{44}$Ca(p,2n)$^{43}$Sc nuclear reactions

Figs. (1-a,b) show the calculated excitation functions for the nuclear reactions $^{44}$Ca(p,n)$^{44m,g}$Sc and $^{44}$Ca(p,2n)$^{43}$Sc in comparison with the available experimental data. The excitation function for the reaction $^{44}$Ca(p,n)$^{44m}$Sc shows the maximum value of about 750 mb and a broad hump within the range 6-14 MeV (Figure 1-a). The data of Mitchell et al.\textsuperscript{(23)}, Levkovskij\textsuperscript{(24)} and De Waal\textsuperscript{(25)} show a roughly good agreement with the theoretical results. The results of Levkovskij\textsuperscript{(24)} were normalized by a factor of 0.82 as indicated by Qaim et al.\textsuperscript{(26)} and Azzam et al.\textsuperscript{(27)}. The data for Krajewskij et al.\textsuperscript{(28)} have a slight energy shift for the thresholds and the peak position. Since the threshold of the $^{44}$Ca(p,2n)$^{43}$Sc reaction is 14.5 MeV, the impurity from $^{43}$Sc isotope can be avoided if the incident beam is less than this value. The presented graphs showed that the results of the two computer codes for the above mentioned reactions are in a good agreement with each other. This may be due to using the similar model parameters for these reactions.

The cross section of the $^{44}$Ca(p,n)$^{44m}$Sc process have low values as shown in Fig. 1-b. TALYS and EMPIRE codes calculations give nearly the same results for the $^{44}$Ca(p,n)$^{44m}$Sc process which are slightly lower than the experimental data in the studied energy range. The data of Krajewskij et al.\textsuperscript{(28)} showed a significant shift in the reaction threshold and high cross section value at 18 MeV in (see Fig. 1-b).
3.1.2 $^{45}$Sc(p,n)$^{45}$Ti and $^{45}$Sc(p,2n)$^{44}$Ti processes

Figs. (2 and 3) show the results of nuclear model calculations for the $^{45}$Sc(p,n)$^{45}$Ti and $^{45}$Sc(p,2n)$^{44}$Ti processes together with the available experimental data within the studied proton energy range as reported in previous studies $^{24, 29-36}$. From the presented graphs, it can be noticed that the formation cross section of the $^{45}$Ti shows a wide peak in the energy range 6-18 MeV. A reasonable agreement between the theoretical and experimental results is observed. The same graph presents a
suggested recommended trend curve for the $^{45}\text{Sc}(p,n)^{45}\text{Ti}$ excitation function. On the other hand, the nuclear reaction $^{45}\text{Sc}(p,2n)^{44}\text{Ti}$ presented in Fig. (3) has much lower cross section values around 23 MeV. The data of Mcgee et al. are very higher than the theoretical and the other experimental curves and therefore they were excluded from our recommended trend curve of the reaction cross section. It is found that TALYS and EMPIRE data are higher than the experimental values of the reaction $^{45}\text{Sc}(p,n)^{45}\text{Ti}$ at low energy region (12-25 MeV), while they are in fairly good agreement with that of $^{45}\text{Sc}(p,n)^{45}\text{Ti}$ reaction. From the two graphs presented in Fig. (2 and 3), one can conclude that the short half-life of $^{45}\text{Ti}$ ($T_{1/2}=3.08\text{h}$) with respect to $^{44}\text{Ti}$ ($T_{1/2}=63\text{y}$) insures the possibility of obtaining pure $^{44}\text{Ti}$ after several hours from EBO even there is some interference between the two formation cross sections.

3.2 Deuteron induced reactions

3.2.1 $^{44}\text{Ca}(d,2n)^{44m}\text{Sc}$ and $^{44}\text{Ca}(d,3n)^{43}\text{Sc}$.

The cross section for production of $^{44}\text{Sc}$ radioisotope through the nuclear reaction $^{44}\text{Ca}(d,2n)^{44}\text{Sc}$ was found to be of the maximum value 500 mb at 15 MeV as shown in Fig.( 4). There is only one set of available experimental data by Duchemin et al. 2015 (35) which is found to be deviated from the TALYS and EMPIRE in the case of $^{44}\text{Sc}$ above 15 MeV. It was also noticed that the excitation function for the formation of the metastable state $^{44m}\text{Sc}$ through the $^{44}\text{Ca}(d,2n)^{44m}\text{Sc}$ reaction is of higher cross section values than the theoretical calculations above proton energy of 15 MeV. Moreover, the EMPIRE results have a satisfactory agreement with the experimental data. There is a slight disagreement between EMPIRE and TALYS curves. The excitation function of the $^{44}\text{Ca}(d,3n)^{43}\text{Sc}$ reaction showed a wide peak over the range 30-50 MeV, where some small part is interfering with the curves of the $^{44}\text{Ca}(d,2n)^{44}\text{Sc}$ and $^{44}\text{Ca}(d,2n)^{44m}\text{Sc}$ reactions from 20 to 30 MeV.

The calculated cross sections of deuteron induced reactions on enriched $^{43}\text{Ca}$ showed a monotonic increasing function with increasing the deuteron energy up to 4 MeV then a semi hump profile is noticed up to 10 MeV as presented in Figs. (5 and 6). The data of De Waal et al. 1971 (25) are of lower values than that of the theoretical calculations. The curves of TALYS and EMPIRE were found to be of the same trend, but some noticeable deviation in the value was found at all the studied energy ranges.

![Graph](image)(2): Excitation function of the proton induced nuclear reaction $^{45}\text{Sc}(p,n)^{45}\text{Ti}$.
Fig. (3): Excitation function of the proton induced nuclear reaction \(^{45}\text{Sc}(p,2n)^{44}\text{Ti}\).

Fig. (4): Excitation functions for the nuclear reactions \(^{44}\text{Ca}(d,2n)^{44m,44g}\text{Sc}\) and \(^{44}\text{Ca}(d,3n)^{43}\text{Sc}\).
3.2.2 $^{45}$Sc(d,2n)$^{45}$Ti, $^{45}$Sc(d,3n)$^{44}$Ti processes

The calculated cross section of deuteron interaction with $^{45}$Sc is presented in Fig. (7) which indicates that the production of $^{45}$Ti radioisotope is theoretically possible within the deuteron energy range 20–50 MeV. It can be noticed that there is a considerable interference between the two nuclear reactions $^{45}$Sc(d,2n)$^{45}$Ti and $^{45}$Sc(d,3n)$^{44}$Ti which allows traces of $^{45}$Ti in the final product of $^{44}$Ti which can be neglected after several hours from EOB. There is only one experimental data set that was reported by Hermann et al., 2012 (38) for the investigated nuclear reactions. It is noticed that the experimental data points are lower than TALYS in the case of the reaction $^{45}$Sc(d,3n)$^{44}$Ti and higher in case of the nuclear reaction $^{45}$Sc(d,2n)$^{45}$Ti at energies higher than 10 MeV. The EMPERE results were found to be in a good agreement with the experimental data for the $^{45}$Sc(d,3n)$^{44}$Ti reaction and much lower in case of $^{45}$Sc(d,2n)$^{45}$Ti nuclear reaction.
Fig. (7): Excitation function of the deuteron induced nuclear reactions $^{45}\text{Sc}(d,3n)^{44}\text{Ti}$ and $^{45}\text{Sc}(d,2n)^{45}\text{Ti}$

Fig. (8): Excitation functions of $\alpha$-particles induced reactions on $^{42,43,44}\text{Ca}$ for production of $^{44}\text{Sc}$
Fig. (9): Excitation functions of α-particles induced reactions on $^{42,43,44}$Ca for production of $^{44m}$Sc.

3.3 α-particle induced reactions

3.3.1 Nuclear reactions on $^{40}$Ca, $^{42,43}$Ca, $^{44}$Ca and $^{44}$Ca

Figs.(8 and 9) present excitation functions for the α-particle induced reactions on $^{42}$Ca, $^{43}$Ca and $^{44}$Ca isotopes for production of $^{44m}$Sc. It is clear that the experimental data of Levkovskij (24) are in a good agreement with TALYS data for the ($\alpha$,np), ($\alpha$,2np) reactions and far from both EMPIRE and TALYS for ($\alpha$,3np) reaction. Furthermore, the results of TALYS and EMPIRE calculations are completely in disagreement with each other for the $^{44g}$Sc and $^{44m}$Sc formation reactions.

The calculated cross section data of $^{40}$Ca(α,p)$^{43}$Sc reaction are plotted in Fig. (10) together with the experimental data of Levkovskij (24) and Howard et al. (29). The experimental data are in disagreement over all the energy range. The data of Howard et al. are consistent and in a good agreement with EMPIRE curve. More experiments are needed in this energy range for satisfactory cross section evaluation. The maximum cross section values are about 700-900 mb around 15 MeV. The data obtained by TALYS calculations were found to be in a good agreement with the results of Levkovskij (24) while the EMPIRE data are very close to that of Howard et al. (29).

3.3.2 $^{43}$Ca(α,xn)$^{44,45}$Ti, $^{44}$Ca(α,xn)$^{44,45}$Ti processes

The calculated cross section data of the nuclear reactions $^{43}$Ca(α,xn)$^{44,45}$Ti and $^{44}$Ca(α,xn)$^{44,45}$Ti are plotted in Figs. (11 and 12). Although there are no any previously reported experimental data for these nuclear reactions, we present the theoretical excitation function as a comparison with the direct routes. The presented curves of the excitation functions showed a very significant overlap between the reactions producing $^{44}$Ti and $^{45}$Ti in a wide energy range (25 – 70 MeV). Furthermore, there are lots of differences between the TALYS and EMPIRE calculated cross section values which result in uncertain integral yields.
Fig. (10): Excitation functions of α-particle induced reaction $^{40}$Ca(α,p)$^{43}$Sc.

Fig. (11): Excitation functions of α-particle induced nuclear reactions $^{43}$Ca(α,xn)$^{44,45}$Ti.

Fig. (12): Excitation function of the α-particle induced nuclear reactions $^{44}$Ca(α,xn)$^{44,45}$Ti.
Fig. (13): The calculated integral yield of the investigated nuclear reactions

4. Integral yield

The calculated and experimental values of the $^{44}$Sc and $^{44}$Ti radioactive yields are given in Table 2. A histogram representation of the calculated values is also presented in Fig. (13) for comparison. We emphasize here that the calculations were normalized to one hour irradiation and 1 µA incident beam, while every corresponding experimental value is given as it is stated in literature without any normalization (9,10,16,17,39). The results revealed that the highest yield of $^{44}$Sc radioisotope can be obtained from the direct routes $^{44}$Ca(p,n)$^{44g}$Sc (1200 MBq/µA.h), $^{44}$Ca(d,2n)$^{44g}$Sc (1083 MBq/µA.h) and $^{44}$Ca(α,3np)$^{44g}$Sc (458 MBq/µA.h), assuming that the targets are of enriched isotopic contents of $^{44}$Ca. The selected energy range for $^{44}$Sc production may eliminate $^{43}$Sc impurity from the final product. The $^{44m}$Sc/$^{44g}$Sc generator should be taken into consideration due their simultaneous existence in the target at EOB. The produced yield of $^{44g}$Sc is normally higher than $^{44m}$Sc due to the large difference in half-lives (58 h and 3.9 h, respectively). The evaluated percentage of the $^{44m}$Sc activity relative to $^{44m+g}$Sc product was found to be less than 15% in most of the reported production experiments (40). The deuteron found to be a good alternative of the proton for nuclear reactions producing no-carrier added $^{44}$Sc with a high radioactive yield (1110 MBq/µA.h) through the (d,2n) nuclear reaction on enriched $^{44}$Ca target.
Table (2): Calculated and experimental yields for the investigated nuclear reactions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Range (MeV)</th>
<th>Calc. yield (MBq/μA.h)</th>
<th>Exp. yield and conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{44}\text{Ca}(p,n)^{44}\text{Sc}$</td>
<td>15→5</td>
<td>1200</td>
<td>1900 MBq/50 μA Enriched $^{44}\text{Ca}$CO$_3$ powder (10 mg) pressed with graphite inside target holder, 50 μA 11 MeV protons for 60-90 min [39]</td>
</tr>
<tr>
<td>$^{44}\text{Ca}(p,2n)^{44}\text{Sc}$</td>
<td>25→15</td>
<td>108</td>
<td>350 MBq/50 μA Enriched $^{44}\text{Ca}$CO$_3$ (10 mg) powder pressed on graphite disc, protons of 17.6 MeV at a beam current of 50 μA for 30–40 min [10].</td>
</tr>
<tr>
<td>$^{44}\text{Ca}(d,n)^{44}\text{Sc}$</td>
<td>8→0</td>
<td>200</td>
<td></td>
</tr>
<tr>
<td>$^{44}\text{Ca}(p,2n)^{44}\text{Sc}$</td>
<td>17→10</td>
<td>1110</td>
<td>44 MBq/0.2 μA.h Enriched $^{44}\text{Ca}$CO$_3$ (100 mg) pressed in pellet from, 16.4 MeV deuterons, beam current 200 nA, 60 min irradiation time [14]</td>
</tr>
<tr>
<td>$^{43}\text{Ca}(d,n)^{44}\text{Sc}$</td>
<td>40→28</td>
<td>452</td>
<td></td>
</tr>
<tr>
<td>$^{43}\text{Ca}(d,2n)^{44}\text{Sc}$</td>
<td>20→8</td>
<td>168</td>
<td>28.9 MBq/0.5 μA Enriched $^{40}\text{Ca}$CO$_3$(100 mg) pellet were irradiated for 30 min by an alpha beam of 20 MeV with beam current of 0.5 μA [16]</td>
</tr>
<tr>
<td>$^{43}\text{Ca}(\alpha,p)^{43}\text{Sc}$</td>
<td>45→20</td>
<td>229</td>
<td>31 MBq/μA·h Enriched $^{42}\text{Ca}$CO$_3$ (68%) , alpha particles energy 29 MeV [17].</td>
</tr>
<tr>
<td>$^{43}\text{Ca}(\alpha,2n)^{43}\text{Sc}$</td>
<td>50→30</td>
<td>226</td>
<td></td>
</tr>
<tr>
<td>$^{43}\text{Ca}(\alpha,3n)^{44}\text{Sc}$</td>
<td>60→40</td>
<td>332</td>
<td></td>
</tr>
<tr>
<td>$^{43}\text{Ca}(\alpha,4n)^{44}\text{Sc}$</td>
<td>60→45</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>$^{45}\text{Sc}(p,2n)^{44}\text{Ti}$</td>
<td>30→15</td>
<td>1.2E-03</td>
<td>Five mCi (150 MBq) of $^{44}\text{Ti}$ were produced utilizing the $^{45}\text{Sc}(p,2n)^{44}\text{Ti}$ process. 1.5 g Sc target was irradiated with an internal proton beam of $E_p \approx 25$ MeV and beam current of 200 μA. [9].</td>
</tr>
<tr>
<td>$^{45}\text{Sc}(p,n)^{45}\text{Ti}$</td>
<td>20→2</td>
<td>429</td>
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<tr>
<td>$^{45}\text{Sc}(d,3n)^{45}\text{Ti}$</td>
<td>50→20</td>
<td>9.4E-05</td>
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</tr>
<tr>
<td>$^{45}\text{Sc}(d,2n)^{45}\text{Ti}$</td>
<td>30→5</td>
<td>695</td>
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<tr>
<td>$^{45}\text{Ca}(\alpha,4n)^{45}\text{Ti}$</td>
<td>90→50</td>
<td>3.0E-05</td>
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<tr>
<td>$^{45\text{Ca}(\alpha,3n)^{45}\text{Ti}}$</td>
<td>60→30</td>
<td>117</td>
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</tr>
<tr>
<td>$^{45}\text{Ca}(\alpha,2n)^{45}\text{Ti}$</td>
<td>60→40</td>
<td>2.7E-04</td>
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<tr>
<td>$^{45}\text{Ca}(\alpha,2n)^{45}\text{Ti}$</td>
<td>50→20</td>
<td>208</td>
<td></td>
</tr>
</tbody>
</table>

The comparison of the yield obtained from the direct production routes and that from indirect processes through $^{44}\text{Ti}/^{44}\text{Sc}$ generator is based on some decay information for the two radionuclides $^{44}\text{Ti}$ and $^{44}\text{Sc}$. As the parent radionuclide $^{44}\text{Ti}$ decays, the concentration of the daughter nucleus $^{44}\text{Sc}$ increases and reaches the maximum after about several hours. The separation process depends on the difference in the chemical properties between parent and daughter elements to flush out the daughter atoms from the generator composite. After isolation of the $^{44}\text{Sc}$ from the generator, its concentration in the medium immediately starts to increase again. The increase in the daughter activity starts to be slow after certain limit of time. Eventually the daughter activity is produced at a rate that nearly equals that
at which it decays. When the ratio of the rate of production of the daughter and its rate of decay stabilize, the system is said to be in equilibrium. After several separation processes the supply of parent product will deplete to insufficient levels and a fresh generator system should be supplied. The daughter activity can be calculated from the following formula:

$$A_{Sc} = \frac{\lambda_{Sc}}{\lambda_{Ti}} A_{Ti} (1 - e^{-(\lambda_{Sc} - \lambda_{Ti})t})$$ (1)

where, $\lambda_{Ti}$ and $\lambda_{Sc}$ are the decay constants of $^{44}$Ti and $^{44}$Sc, respectively, and $t$ is the elapsed time after production. If $\lambda_{Ti} \ll \lambda_{Sc}$ i.e. the half-life of the daughter is much shorter than the half-life of its parent, we have:

$$A_{Sc} = A_{Ti} (1 - e^{-\lambda_{Sc}t})$$ (2)

In general, it is not practical to wait until radioactive equilibrium has been reached before the isolation of the daughter nucleus. By setting $t = T_{1/2} (Sc)$ into Eq. (2), we obtain:

$$A_{Sc} = A_{Ti} (1 - e^{-ln2}) = 0.5 A_{Ti}$$ (3)

This means that we can obtain 50% of the produced activity after a growing-in time of one daughter half-life. However, the reported experimental data bear more details that should be under focus. It was reported that a stock of $^{44}$Ti solution with 30 kBq was prepared from Sc target irradiated by 25 MeV protons $^{8}$. The total activity from the $^{43}$Sc(p,2n)$^{44}$Ti nuclear reaction was 150 MBq/ 200 $\mu$A (5 mCi). The reported $^{44}$Sc activity after several fractions of isolation from the Ti solution reached 60 MBq $^{8,9}$ which is about 40 % of the original activity of the target which is in agreement with calculations.

Retuning to the calculated yield obtained from the proton or deuteron induced reactions on the Sc, it was noticed that the produced activity of $^{44}$Ti is lower than that of $^{45}$Ti due to the difference in the half lives of both radionuclides. One can conclude that special precautions should be taken into consideration in production of $^{44}$Ti, where using the product can be delayed until low activity of $^{45}$Ti is achieved. On the other hand, it is noticed that direct production routes are producing a higher yield value especially the proton induced reaction on enriched $^{44}$Ca ($1213$ MBq/ $\mu$Ah). The choice of the suitable method for production of $^{44}$Sc depends on the selected separation method. Furthermore, transportation time is an effective factor for the delivered activity for medical usage because the $^{44}$Sc is of a short half-life (3.9 h) and therefore, in some cases the $^{44}$Ti/$^{44}$Sc generator method would be preferred for long transportation time.

5. CONCLUSIONS

The present study covers most of the direct and indirect production routes for the production of the $^{44}$Sc radioisotope. The nuclear models calculation confirmed some of the reported experimental cross section values within the studied range of energy. Some necessary improvement on the nuclear model codes TALYS and EMPIRE are needed to resolve the significant disagreement with experimental data of some nuclear reactions. Additional experiments are also needed for validation of the theoretical results, especially in the case of $d$ and $\alpha$-particle induced reactions. The results revealed that production of the $^{44}$Ti can be done with low yield using proton beam. Furthermore, the deuteron and $\alpha$-particle induced reactions lead to much lower yield values than those for proton (3-5 order less).

REFERENCE


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