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SIMULATION OF VANADIUM-48 PRODUCTION USING MCNPX CODE

by

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Vanadium-48 was produced through the irradiation of the natural titanium target via the $^{nat}Ti(p, xn)^{48}V$ reaction. The titanium target was irradiated at 1 A current and by a 21 MeV proton beam for 4 hours. In this paper, the activity of ^{48}V, ^{43}Sc, and ^{46}Sc radionuclides and the efficacy of the $^{47}Ti(p,)$, $^{48}Ti(p, n)$, and $^{49}Ti(p, 2n)$ channel reactions to form ^{48}V radionuclide were determined using MCNPX code. Furthermore, the experimental activity of ^{48}V was compared with the estimated value for the thick target yield produced in the irradiation time according to MCNPX code. Good agreement between production yield of the ^{48}V and the simulation yield was observed. In conclusion, MCNPX code can be used for the estimation of the production yield.

Key words: activity, MCNP code, natural titanium, vanadium-48

INTRODUCTION

Positron emission tomography (PET) is a non-invasive medical imaging technology that can generate high resolution images of physiologic functions with clinical application for oncology, cardiology, and neurology [1]. Formerly, the majority of the PET centers used to employ ^{68}Ge ($T_{1/2}$ = 271 d) in equilibrium with ^{68}Ga for routine transmission scanning. In order to improve the quality of PET images by acquiring high count and short duration transmission scans, the positron emitter ^{48}V ($T_{1/2}$ = 15.97 d; β^+ decay 50% and γ-line: 944.13, 983.52, and 1312.10 keV) [2] that can be presented by many PET cyclotrons, is an interesting candidate for PET imaging [2-6].

^{48}V is frequently used in nuclear medicine; for example, the ^{48}V radioactive stent was produced by a nickel-titanium stent irradiation with the proton beam, and the efficacy of radioactive stent for application in renal artery brachytherapy was studied [7].

Titanium, a light, strong, non-toxic metal, has a wide array of practical applications in the field of industry and aerospace. Its physical and chemical properties, together with an unrestricted availability make titanium an ideal target material for monitoring beam parameters. Therefore, the $^{nat}Ti(p, x)^{48}V$ is a suitable reaction for monitoring the intensity and energy of charged particle beams [2, 6, 8]. The use of monitor reaction is a convenient and cheep method for determining the energy and intensity of the bombarding beam.

Production of ^{48}V by natural titanium, has been studied via the $^{nat}Ti(p, xn)$ [2-9], $^{nat}Ti(d, xn)$ [4] and $^{nat}Ti(\alpha, xn)$ [10] reactions. The $^{nat}Ti(p, xn)^{48}V$ reaction is suitable for medium to low-energy cyclotrons. Table 1 shows the nuclear data of ^{48}V production through the different isotopes of natural Ti using TALYS code.

Moreover, Ti is a potential candidate for the production of medical radionuclides, such as ^{48}V, ^{43}Sc, ^{46}Sc, and so on. The positron emitting radionuclide ^{43}Sc ($T_{1/2}$ = 3.89 h; E_γ = 372.8 keV) could be used for *in vivo* dosimetry [11] and ^{46}Sc radionuclide was used as a radiotracer to analyze lungs [12]. Therefore, the

Table 1. Nuclear data ^{48}V production through different isotopes of natural Ti using TALYS code

Contributing reactions	Q-value [MeV]	Threshold [MeV]	Abundance of target nucleus [%]
$^{47}Ti(p,)^{48}V$	6.83	0	7.3
$^{48}Ti(p, n)^{48}V$	−4.79	4.89	73.8
$^{49}Ti(p, 2n)^{48}V$	−12.93	13.20	5.5
$^{50}Ti(p, 3n)^{48}V$	−23.88	24.36	5.4

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^{nat}Ti(p, x)^{48}V, ^{43,46}Sc nuclear processes have great importance in the field of nuclear medicine.

In this work, production of radionuclide through the ^{nat}Ti(p, x) reaction, was simulated using Monte Carlo code. In this simulation, the natural Ti – ^{46}Ti (8.0%), ^{47}Ti (7.3%), ^{48}Ti (73.8%), ^{49}Ti (5.5%), and ^{50}Ti (5.4%) – was irradiatedat 10 A current and 21 MeV proton beam, with 10 million proton histories. The computer code MCNPX was chosen to simulate the proton flux in the natural Ti and determined the radionuclide activity. The comparison study was made between experimental and theoretical of the ^{48}V activity and the calculated values based on the simulated proton flux.

MATERIALS AND METHODS

Calculation of excitation function

The TALYS code: The pre-equilibrium particle emission is described using the two-component exciton model. The model implements new expressions for internal transition rates and new parameterization of the average squared matrix element for the residual interaction obtained using the optical model potential. The phenomenological model is used for the description of the per-equilibrium complex particle emission. The equilibrium particle emission is described using the Hauser-Feshbach model [13].

Excitation functions of ^{nat}Ti(p, x)^{48}V reaction were calculated by using TALYS 1.0 code.

TALYS 1.0 is a computer code system for the analysis and prediction of nuclear reactions. The basic objective behind its construction is the simulation of nuclear reactions that involve neutrons, photons, protons, deuterons, tritons, ^{3}He-particle, and alpha particles in the 1 keV-200 MeV energy [13]. The good agreement between most of the literature data and data from the TALYS code was observed [2, 6, 8].

Excitation functions calculated by TALYS-1.0 code are shown in fig. 1 at different decay channels after proton bombardment of natural titanium. As seen in fig. 1, the optimum bombarding energy range is
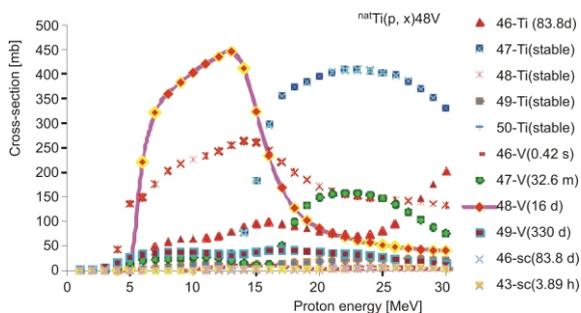
Figure 1. The excitation function of ^{nat}Ti(p, x) reaction

8-20 MeV, with the maximum cross-section of 464 mb (1 mb = 10^{-31}m^2) at 13 MeV. The reactions lead to the formation of ^{46}Ti, $^{46/47/48/49}$V, and $^{43/47}$Sc activity impurities.

Non-isotopic contaminations can be separated by virtue of chemical methods and the isotopic impurities ^{46}V and ^{47}V were not notable, since their half-lives are extremely short (0.46 s and 32.6 m) and ^{49}V has a very small cross-section in the 8-20 energy range.

The excitation function of ^{48}V on natural Ti through the ^{47}Ti(p, γ), ^{48}Ti(p, n), ^{49}Ti(p, 2n), and ^{50}Ti(p, 3n) nuclear reactions using the TALYS code, is shown in fig. 2.

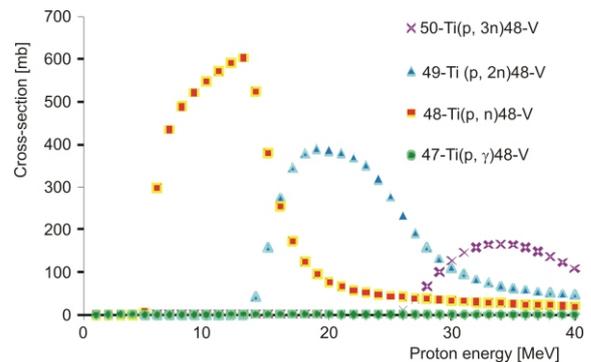**Figure 2. The excitation function production of ^{48}V on natural Ti**

According to the SRIM (The Stopping and Range of Ions in Matter) code, the required thickness of the target was calculated for any reaction [14]. The physical thickness of the Ti layer (0.11 cm) is chosen in such a way that for a given beam/target angle geometry (90°) the incident beam of the target layer be excited with the predicted energy.

Calculation of theoretical yield using TALYS and SRIM cods

Analytical estimation of the theoretical activity production were made utilizing the evaluated cross-section data from the ^{nat}Ti(p, x) using TALYS code and the stopping power calculated using SRIM code. The production yield Y (in Bq) can be calculated by the Simpson numerical integral method from eq. (1).

$$Y \quad \frac{N_L H}{M} I(1 \quad e^{\quad \lambda t}) \int_{E_1}^{E_2} \frac{d(\rho x)}{dE}^{\quad 1} \sigma(E) dE \quad (1)$$

where N_L is the Avogadro number, H – the isotope abundance of the target nuclide, M – the mass number of the target element, $\sigma(E)$ – the cross-section at energy E, I – the projectile current, $dE/d(\rho x)$ – the stopping power, and λ – the decay constant of the product and t – the time of irradiation [15-20].

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Calculation of simulation yield using the Monte Carlo

MCNP (Monte Carlo N-particle) is a general purpose Monte Carlo radiation transport code developed by Los Alamos National Laboratory (LANL) and designed to track many particle types such as neutron, photon, electron, or coupled (neutron/photon/electron) over broad ranges of energies [21].

Afterward, the code has been under a constant development, latest and most advanced version is called MCNPX. The MCNPX code extends the capabilities of MCNP4C3 to nearly all particle types, to nearly all energies, and to nearly all applications without an additional computational time penalty. The MCNPX code is capable of simulating 34 particle types and more than 2000 heavy ions at low as well as high energies. It utilizes the latest nuclear cross-section libraries and uses physics models for particle types.

The MCNPX input file included information such as: the geometry, the description of materials, the type tallies, source, and the variance reduction techniques.

The target cell was defined as volume of space bounded by surfaces. The target consisting of a titanium cylinder (height = 0.11 cm; radius = 0.50 cm) enveloped in high purity Al foil (16 m thick). The bottom of the cylinder was located in the plane $Z = 0$ and the cylinder axis is parallel to Z axis. fig. 3(a) shows the model of target and source.
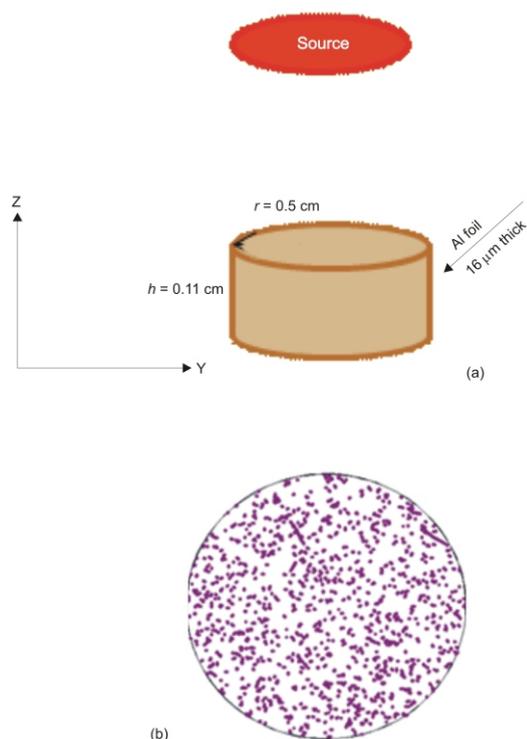

(a)

(b)

Figure 3.
*(a) – schematic of the target and source, and (b) – surface of ^{nat}Ti target, irradiated with 1000 protons, designed with visual editor MCNP**X***

The source was specified by the SDEF command. The SDEF command has many variables or parameters that are used to define all the characteristics of all sources. In this work, SDEF card simulated a pulse of proton beam with 21 MeV energy and $I = 10$ A, around the Z axis with a negative direction. The simulated proton beam has an annular shape (Ø = 1 cm, $R_{min} = 0$, $R_{out} = 0.5$ cm). Figure 3(b) shows the surface of natural Ti target was irradiated with 1000 protons, by using the Visual Editor MCNPX.

Proton flux (F4 and F4/e4) was calculated using MCNPX version 2.6 and particle distribution functions $P(E)$ was computed from F4 tally data that were normalized over the entire particle energy range.

The ^{nat}Ti(p, x)^{48}V,^{43,46,47}Sc published cross-section data, and the MCNPX proton flux distributions have a proton energy dependence. All the cross-section spectra and the proton flux were divided in a series of 0.5 MeV energy regions. These energy regions are small enough that the average cross-section and the proton flux values are considered constant for each region.

The calculation of instable product nuclide was based on expression

$$A(t) = \int_0^{E_{max}} P(E)\sigma(E)\,\mathrm{d}E \frac{\mathrm{d}N_p}{\mathrm{d}t}\,d\rho\frac{L}{M}(1 - e^{-\lambda t}) \quad (2)$$

where $A(t)$ is the product nuclide radioactivity, λ – the decay constant of the product isotope, L – the Avogadro constant, M – the target material molar, ρ – the target material density, d – the target thickness, $I = = \mathrm{d}N_p/\mathrm{d}t$ – the proton beam current, and t – the irradiation time. The product function $P(E)\sigma(E)$ was computed from cross-section multiplying polynomial fits of 5th degree of the particle distribution functions based on the MCNPX code. Figure 4 shows the normalized energy distribution function $P(E)$ for proton in the Ti cell.
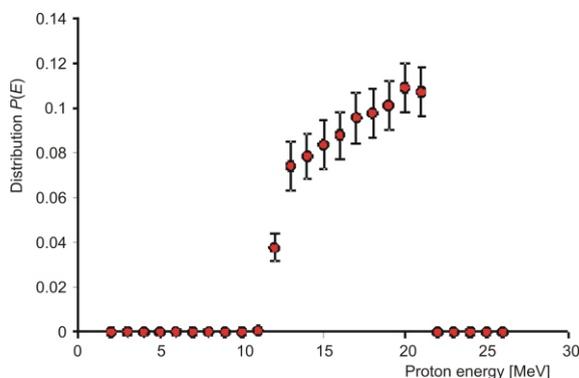

Figure 4. Normalized energy distribution function for the proton in the natural titanium given by MCNPX

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RESULTS AND DISCUSSION

Theoretical production yield – TALYS and SRIM codes

Natural titanium was used as the target for the irradiation, but formation of the ^{48}V radionuclide in 20-8 MeV energy range is only contributed to by several direct reactions: the ^{47}Ti(p, γ), ^{48}Ti(p, n), and ^{49}Ti(p, 2n). The reaction channel ^{50}Ti(p, n)^{48}V, did not contribute significantly, since their starting energy is >20 MeV (see fig. 2). The yield of ^{48}V through the ^{47}Ti(p, γ)^{48}V and ^{49}Ti(p, 2n)^{48}V reactions, are very small (0.004 and 0.7 MBq/ Ah). The theoretical production yield ^{48}V via the ^{nat}Ti(p, n)^{48}V reaction was calculated 21.18 MBq/ Ah.

Simulation production yield – MCNPX code

The estimated experimental value for the yield production ^{48}V in 4 hours of irradiation at 10   is calculated 22.25 MBq/ Ah at the end of the bombardment [3].

The production of the ^{48}V yield in the simulated 10 10^6 proton histories is evaluated as 22.17 MBq/ Ah. Table 2 shows a comparison between the theoretical and experimental activity of ^{48}V with the calculation activity based on the proton flux distributions on the natural Ti using the simulation code MCNPX, through the ^{nat}Ti(p, x)^{48}V reaction.

Table 2. Comparison between the theoretical activity, the experimental activity and the calculation ^{48}V activity based on MCNPX

Reoretical	Theoretical activity [MBq]	Experimental activity [3] [MBq]	Simulation activity [MBq]
^{nat}Ti(p, x)^{48}V	847.23	890	886.87

The production radionuclide contaminants were calculated using the MCNPX. The simulation of production ^{43,46}Sc in the Ti can be estimated respectively, as 11.22, and 0.019 MBq/ Ah. The contributions to the impurities radionuclide could be eliminated using 100% isotopically enriched ^{48}Ti target instead of natural Ti. The simulation yield of ^{48}V through the ^{47}Ti(p, γ)^{48}V and ^{49}Ti(p, 2n)^{48}V reactions, are 0.005 and 1.02 MBq/ Ah based on the MCNPX code.

Table 3 shows the production of radionuclide ^{48}V and ^{43,46}Sc through the ^{nat}Ti(p, x) reaction and

Table 3. Comparison between the theoretical yield and the calculation based on MCNPX

Radionuclide	^{48}V	^{43}Sc	^{46}Sc
Theoretical yield [MBq/ Ah	21.18	9.60	0.012
Simulation yield [MBq/ Ah	22.17	11.22	0.019

comparison between theoretical yield and calculation based on the MCNPX code.

CONCLUSIONS

In this work, the simulation code (MCNPX) was used to estimate the activity ^{48}V and contaminants radionuclide through the ^{nat}Ti(p, x) reaction. The ^{48}V activity through the ^{nat}Ti(p, x)^{48}V reaction was almost equal to the activity data from the ^{48}Ti(p, x)^{48}V reaction, because the ^{48}Ti(p, n) (^{48}Ti: 73.8% in natural Ti) reaction is the dominant process for production of ^{48}V using natural Ti.

Good agreement obtained between the theoretical and experimental data of the radionuclide activity, and the calculated activities based on the MCNP proton flux. This comparison demonstrated that the MCNPX provides a suitable tool for simulation of proton irradiation for the purpose of radionuclide production.

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Махди САДЕГИ, Махбобех МАХМОДИ, Тајеб КАКАВАНД, Клаудио ТЕНРЕИРО

СИМУЛАЦИЈА ПРОИЗВОДЊЕ ВАНАДИЈУМА-48 УПОТРЕБОМ MCNPX ПРОГРАМА

Ванадијум-48 производи с е озрачивањем природног титанијума путем реакције ^{nat}Ti(p, xn)^{48}V. Титанијумска мета зрачена је 4 сата протонским снопом енергије 21 MeV, при јачини струје од 10   А. У овом раду, коришћењем програма MCNPX утврђене су активности радионуклида ^{48}V, ^{43}Sc и ^{46}Sc, као и ефикасности реакција канала ^{47}Ti(p, g), ^{48}Ti(p, n) и ^{48}Ti(p, 2n) ради формирања ^{48}V. Експериментално одређена активност ^{48}V поређена је са процењеном вредношћу за принос дебеле мете према MCNPX програму. Уочена су добра слагања приноса производње и симулираног приноса ^{48}V, одакле се закључује да се MCNPX програм може користити за процену приноса производње.

Кључне речи: акｔивносｔ, MCNP ｐроｇрам, ｐриродни ｔиｔанијум, ^{48}V