



## Calculation of Production Reaction Cross Section of Some Radiopharmaceuticals Used in Nuclear Medicine by New Density Dependent Parameters

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**Abstract:** In nuclear medicine, radiopharmaceuticals are used for diagnosis or treatment purposes. Radiopharmaceuticals containing radionuclide in their structure are produced by reactors, generators or cyclotrons and are generally used for scintigraphy or tomographic investigations. The produced radionuclides can be given to the human body together with organic or inorganic substances. In this study, the production reaction cross sections were calculated for two selected radiopharmaceutical nuclei (<sup>99</sup>Tc and <sup>115</sup>In) using the semi-empirical cross section formula for the (n,α) reactions developed by Tel et al. (2008). The density depending on (n, α) reaction cross sections were also investigated with the four Skyrme Hartree Fock parameters (S3, T3, SKM and SKM\*). While the calculated value from the semi-empirical formula developed by Tel et al. (2008) gave reasonable results, the density-dependent calculations were observed lower values than that of experimental values.

**Keywords:** Nuclear medicine, Nuclear reactions, Cross section, Skyrme potential, Asymmetry parameter

## Nükleer Tıpta Kullanılan Bazı Radyofarmasötiklerin Üretim Reaksiyon Tesir Kesitlerinin Yoğunluğa Bağlı Yeni Parametrelerle Hesaplanması

**Özet:** Nükleer tıpta, radyofarmasötikler tanı veya tedavi amacıyla kullanılmaktadır. Yapılarında radyonüklid içeren radyofarmasötikler, reaktör, jeneratör veya siklotronlarla üretilirler ve genellikle sintigrafik veya tomografik incelemelerde kullanılır. Üretilen radyonüklidler, organik veya inorganik maddelerle birlikte vücuda verilebilir. Bu çalışmada, (n, α) reaksiyonları için Tel ve arkadaşları (2008) tarafından geliştirilen yarı-ampirik tesir kesit formülü kullanılarak seçilen iki radyofarmasötik çekirdek (<sup>99</sup>Tc ve <sup>115</sup>In) için üretim reaksiyonu tesir kesitleri hesaplanmıştır. Ayrıca, yoğunluğa bağlı ampirik (n, α) (2008) nükleer reaksiyon tesir kesitleri dört Skyrme Hartree Fock parametreleri (S3, T3, SKM ve SKM\*) kullanılarak da incelenmiştir. Tel ve ark. (2008) tarafından geliştirilen yarı ampirik formülünden hesaplanan değer uyumlu çıkarken, yoğunluğa bağlı hesaplamaların deneysel değerlerden daha aşağıda olduğu gözlemlenmiştir.

**Anahtar kelimeler:** Nükleer tıp, Nükleer reaksiyonlar, Tesir kesiti, Skyrme potansiyeli, Asimetri parametresi

## 1. Introduction

Radiopharmaceuticals are radioactive compounds that do not cause a physiological disturbance when given at appropriate doses and are used for diagnosis-treatment purposes. Radiopharmaceuticals, which are extremely important in the diagnosis of the disease, are formed as a result of combining gamma photon release radioactive substances. These substances that are given to the patient are placed in the target organ, making the target organ a source of radioactive material thanks to the radioactive nuclei in its structure. The production of all radionuclides used in nuclear medicine is made by making stable atoms radioactive by artificial means [1].

Technetium (Tc) element with atomic number 43 is widely used for the diagnosis of decreased coronary perfusion (Myocardial ischemia) and myocardial infarction.  $^{99m}\text{Tc}$  isotope, produced by bombardment of Mo (half-life is 2.75) isotopes, is also used in thyroid, parathyroid, kidneys, bone and some other scintigraphy uses. It emits detectable gamma rays with photon energy of 140 keV and its 93.7% decays to  $^{99}\text{Tc}$  in 24 hours (half-life of 6 hours). For this reason it allows to use for diagnostic purposes.

Indium (In) element with atomic number 49 is used to determine the acceptance of organ transplantation, detection of abdominal infections, antibody labelling and follow-up of the immune system of the body, follow-up of the organ concentration in the liver and kidneys, follow-up of the white blood cells, cell dosimeter, myocardial scans, and the threat of leukemia. In nuclear medicine, the use of  $^{115}\text{In}$  isotope is extremely limited due to being weakly radioactive and ~ 95.7% is stable.

It is the main objective of the radionuclides to be given to the patient and therefore to be applied in the dose which will give the patient the least harm. For this purpose, the radionuclide used to increase the dose of radiation taken by the patient should not emit beta ( $\beta$ ) rays (except for the applications needed for beta radiation treatment such as radiosynovectomy) and half-life should be short. It should also be suitable for chemical bonding with different pharmaceutical agents with high specific activity and in harmony with the gamma energy detection system.

In this study, the production reaction cross sections have been calculated for two selected radiopharmaceutical nuclei ( $^{99}\text{Tc}$  and  $^{115}\text{In}$ ) by using the semi-empirical cross section formula for the (n, $\alpha$ ) reactions developed by Tel et al. [2] combining with the Skyrme Hartree Fock parameters (S3,T3,SKM and SKM\*). The obtained cross sections (in unit of mb) results were given in figures as a function of radii.

## 2. Materials and Methods

Hartree-Fock with active interaction to investigate ground state properties of the core calculations is used and these studies provide important data for understanding effective interaction [3-6]. However, among these interactions, the Hartree-Fock method with the Skyrme interaction is the most suitable for the calculation of the basis condition of all the nuclei from the light nuclei to the heavy nuclei [7]. The simple mathematical structure of the Skyrme interaction provides convenience for the derivation of Hartree-Fock equations. The Skyrme Hartree-Fock method [8] is based on the Shell model, which basically assumes that a nucleon moves independently within the average central potential created by other nucleons. In the frame of Shell model, when the base state of the nuclei  $\varphi_i$  is considered to be represented by a  $\varphi$  Slater determinant of single particle states, these quantities depend on  $\varphi_i$  single particle states which define  $\varphi$  Slater determinant:

$$\varphi(x_1, x_2, \dots, x_A) = \frac{1}{\sqrt{A!}} \det |\varphi_i(x_j)| \quad (1)$$

Where  $x$  represents the coordinates of the  $r$  space,  $\sigma$  spin and  $q$  isospin (for  $q = +1/2$  proton,  $q = -1/2$  neutron), and  $A$  represents the total number of nucleons in the nucleus [9]. The most important advantage of the Skyrme effect is that the Hartree-Fock energy can be written as only three local intensive functions. Density and momentum dependent Skyrme interaction [10], zero-range formation due to Dirac delta function, allowing Hartree-Fock energy to be written as a function of density, and its simple mathematical structure is the advantage of this interaction [11,12]. This interaction with zero-range, density and momentum is written as follows:

$$\begin{aligned} \bar{V}_{\text{Skyrme}} = \sum_{i < j} \bar{V}_{ij} = & t_0(1 + x_0 P_\sigma) \delta(\bar{r}_i - \bar{r}_j) + \frac{1}{2} t_1(1 + x_1 P_\sigma) \cdot \left\{ \delta(\bar{r}_i - \bar{r}_j) \bar{k}^2 \right\} + \bar{k}^2 \delta(\bar{r}_i - \bar{r}_j) \\ & + t_2(1 + x_2 P_\sigma) \bar{k} \cdot \delta(\bar{r}_i - \bar{r}_j) \bar{k} + i t_4 (\bar{\sigma}_i + \bar{\sigma}_j) \cdot \bar{k} \times \delta(\bar{r}_i - \bar{r}_j) \bar{k} + \frac{1}{6} t_3(1 + x_3 P_\sigma) \delta(\bar{r}_i - \bar{r}_j) \cdot \rho^\alpha \left( \frac{\bar{r}_i + \bar{r}_j}{2} \right) \end{aligned} \quad (2)$$

where  $\bar{k} = \frac{1}{2i}(\bar{\nabla}_i - \bar{\nabla}_j)$  and  $\bar{k} = -\frac{1}{2i}(\bar{\nabla}_i - \bar{\nabla}_j)$  acting on the right and left operators of the momentum of nucleon. Relative motion in the initial and final states, is relative momentum,  $\delta(\bar{r}_{ij})$  is the delta function,  $P_\sigma$  is the spin exchange operator,  $\bar{\sigma}$  is the vector of Pauli spin matrices,  $r = (\bar{r}_j - \bar{r}_i)$  and  $\bar{R} = \frac{1}{2}(\bar{r}_i + \bar{r}_j)$  are the relative and center of mass radius vectors of two nucleus, respectively.  $t_0, t_1, t_2, t_3, t_4, x_0, x_1, x_2, x_3$  and  $\alpha$  are Skyrme force parameters describing the strengths of the different interaction terms [12].

In calculation of base state properties containing important information about the structure of the nucleus, the phenomenological forces with adjustable parameters are often used. The most important properties of these forces are simple mathematical structure and setting parameters with experimental data. Skyrme type forces are widely used phenomenological forces in defining the base state properties of nuclei. These forces can be used together with the Hartree-Fock method to calculate the size of nucleus, density distributions, surface thickness, which are very important and experimentally measurable quantities for the core structure analysis. In this study, nuclear neutron and proton densities were calculated theoretically from four selected Skyrme Hartree-Fock [11] parameter sets (S3, T3, SKM, SKM\*) to calculate production reaction cross sections. The density values for each Skyrme parameter set were used in semi-empirical cross section formula developed by Tel et al. [2], putting density values instead of asymmetry parameters.

These formulas are given as follows [2]:

$$\sigma(n, \alpha) = 16.15(A^{1/3} + 1)^2 \exp(-33.01s) \quad \text{for } 20 \leq A \leq 239 \quad (3)$$

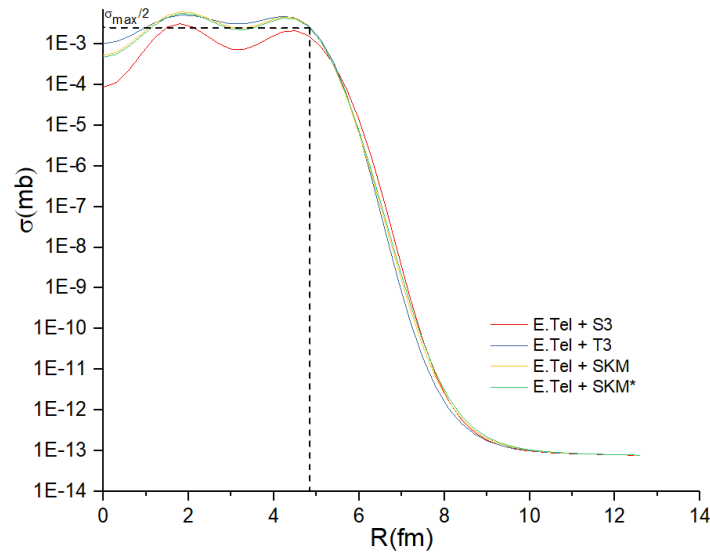
Instead of the  $S = (N-Z/A)$  term given in Eq. (3), the density term given in Eq. (4) is used as follows

$$S = (\rho_n - \rho_p) / (\rho_n + \rho_p) \quad (4)$$

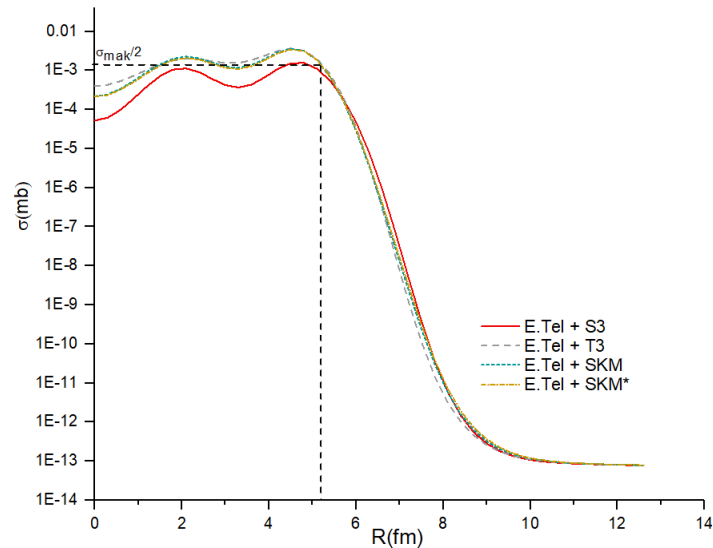
where,  $\rho_n$  and  $\rho_p$  are neutron and proton density.

### 3. Results

Nuclear radiopharmaceuticals used for diagnostic purposes in nuclear medicine must emit enough radiation and have a short half-life to have no effect on the patient body. The radiopharmaceuticals used for this purpose are various isotopes of atoms such as Technetium ( $^{99}\text{Tc}$ ) and Indium ( $^{115}\text{In}$ ) as given in Table 1. The results obtained by semi empirical  $(n, \alpha)$  cross section formula developed by Tel et al. (2008) [2] nuclear reaction formula with the Skyrme Hartree Fock parameters (S3, T3, SKM and SKM\*) are given in Figure 1 and 2. The cross section calculation (in mb unit) as a function of radii for  $^{99}\text{Tc}$  is given in Figure 1. It is clearly seen that the mean half-height value ( $\sigma_{\text{max}}/2$ ) of cross section calculation depending on density is around 4.8 fm radius in Figure 1. Moreover, the cross section calculations depending on density and mean half-height value ( $\sigma_{\text{max}}/2$ ) of  $^{115}\text{In}$  is around 5.1 fm radius can be seen in Figure 2.



**Figure 1.** Theoretical  $(n, \alpha)$  reaction calculations by using Tel et al. [2] formula with the Skyrme Hartree Fock parameters for  $^{99}\text{Tc}$ .



**Figure 2.** The same with Figure 1, but for  $^{115}\text{In}$ .

In Table 1, formation reactions of both nuclei and also density dependent calculations by using Skyrme-Hartree Fock (S3, T3, SKM and SKM\*) parameters have been given, respectively. Additionally, density dependent cross section calculation's mean half-height value ( $\sigma_{\text{max}}/2$ ) can be seen in Table 1 for  $^{99}\text{Tc}$  and  $^{115}\text{In}$  nuclei.

**Table 1.**  $^{99}\text{Tc}$  and  $^{115}\text{In}$  calculations depending on density and  $\sigma_{\text{exp}}$  value between 14-15 MeV (mb unit)

Reaction	$\sigma_{\text{exp}}$	$\sigma_{\text{Tel}}$	$\sigma_{\text{max}/2}$	$\sigma_{\text{Tel+S3}}$	$\sigma_{\text{Tel+T3}}$	$\sigma_{\text{Tel+SKM}}$	$\sigma_{\text{Tel+SKM}^*}$
$^{99}\text{Tc}(n,\alpha)^{96}\text{Nb}$	6.1 ( $\pm 0.6$ )[13]	6.7	$2.4 \times 10^{-3}$	$1.3 \times 10^{-3}$	$2.1 \times 10^{-3}$	$3.1 \times 10^{-3}$	$2.8 \times 10^{-3}$
$^{115}\text{In}(n,\alpha)^{112}\text{Ag}$	2.4 ( $\pm 0.3$ )[14]	0.135	$1.7 \times 10^{-3}$	$7.9 \times 10^{-4}$	$1.8 \times 10^{-3}$	$1.8 \times 10^{-3}$	$1.2 \times 10^{-3}$

#### 4. Conclusion and Comment

Consequently, we proposed a new method of using density values calculated from four Skyrme [12] parameter sets (S3, T3, SKM, SKM\*) instead of the S parameter in semi-empiric formula developed by Tel et al. [2]. In Table 1, the experimental data and the calculated cross section values from Tel formula were compatible for  $^{99}\text{Tc}$ . However, density-dependent calculations were lower than the experimental values.

It is thought that this method can be applied to lighter nuclei, neutron rich nuclei, neutron stars having an important place in astrophysics. And also, through this study, it is possible to investigate the type of basic nucleon-nucleon potentials for the target nuclei by taking advantage of the cross-sections of different reactions. We think that the results obtained from this new density dependent cross section calculation method will contribute to different perspectives in literature.

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