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Reaction Cross Section Calculations in Neutron Induced Reactions and GEANT4 Simulation of Hadronic Interactions for the Reactor Moderator Material BeO

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Abstract: BeO is one of the most common moderator material for neutron moderation; due to its high density, neutron capture cross section and physical-chemical properties that provides usage at elevated temperatures. As it's known, for various applications in the field of reactor design and neutron capture, reaction cross–section data are required. The cross–sections of (n,α), (n,2n), (n,t), (n,EL) and (n,TOT) reactions for ^{9}Be and ^{16}O nuclei have been calculated by using TALYS 1.6 Two Component Exciton model and EMPIRE 3.2 Exciton model in this study. Hadronic interactions of low energetic neutrons and generated isotopes–particles have been investigated for a situation in which BeO was used as a neutron moderator by using GEANT4, which is a powerful simulation software. In addition, energy deposition along BeO material has been obtained. Results from performed calculations were compared with the experimental nuclear reaction data exist in EXFOR.

Reaktör Moderator Malzemesi BeO için Nötron Girişli Reaksiyonlarda Reaksiyon Tesir Kesiti Hesaplamaları ve Hadronik Etkileşimlerin Geant4 Benzetimi

Anahtar Kelimeler
Reaksiyon tesir kesiti,
Hadronik etkileşimler,
Geant4,
TALYS,
EMPIRE,
Berilyum oksit

Özet: BeO; yoğunluğu, nötron yakalama tesir kesiti ve yüksek sıcaklıklarda kullanılmasına imkân veren fiziksel-kimyasal özellikleri sayesinde nötron moderasyonunda oldukça yaygın kullanılan bir moderatör malzemesidir. Bilindiği üzere, reaksiyon tesir kesiti hesaplamaları reaktör tasarımı ve nötron yakalaması alanlarında pek çok çeşitli uygulamalar için gereklidir. Bu çalışmada, ^{9}Be ve ^{16}O için (n,α), (n,2n), (n,t), (n,EL) and (n,TOT) reaksiyonları tesir kesiti hesaplamaları TALYS 1.6 İki Bileşenli Eksiton model ve EMPIRE 3.2 Eksiton modelleri kullanılarak tamamlanmıştır. Güçlü bir benzetim programı olan GEANT4 ile BeO'in nötron moderatörü olarak kullanıldığı bir ortam için düşük enerjili nötronların ve üretilen izotop-parçacıkların hadronik etkileri araştırılmıştır. Ek olarak, BeO malzemesi boyunca enerji birikimi elde edilmiştir. Gerçekleştirilen hesaplamaların sonuçları ayrıca EXFOR veri tabanında yer alan deneysel nükleer reaksiyon verileri ile karşılaştırılmıştır.

1. Introduction

Growing in the population, human needed and technological developments cause day-by-day growing energy consumption. Conventional energy production methods will not be able to cover the request of growing energy demand in clean and safe way. To solve this problem, scientists are still working on one of the possible solutions that is fusion reactors. For a safe design, the development of structural materials and materials microstructure change under the effect of radiation have a great importance.

Neutron moderation is the key for reactors efficiency, stability and energy production rate. The moderation for neutrons have been performed with some materials such as graphite, heavy water, lithium, beryllium and boron for a very long time. Even though these materials serve the neutron moderation purpose well, the current neutron moderators are demanded to work under high temperature, pressure and high efficiently [1]. Further studies shown that

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also composite materials could be used for neutron moderation. One of those materials is the beryllium-oxide, which preferred mostly as a neutron moderator due to its high density, neutron capture cross section and physical-chemical properties makes it usable under previously mentioned situations [2]. The characteristics of beryllium-oxide have been given in Table 1.

Table 1. Characteristics of BeO [2].

Chemical Formula	BeO
Molar Mass	25.01 g.mol^{-1}
Density	3.01 g.cm^{-3}
Melting Point	2507 ^{0}C
Boiling Point	3900 ^{0}C

For fusion reactor technology and its development; neutron induced reaction cross sections data have a critical importance and evaluated values in nuclear databases form that cross sections are used for neutronic interaction computations [3]. Material analysis is the basis of fission and fusion reactor design and this basis depends on the calculated reaction cross sections. Besides, in addition to the importance of the calculated reaction cross section data, it is also important even critical to simulate the events and environment on and over the desired material or part of the reactor/structure. Since it is unavailable to be able to work on a real working fusion reactor, simulation of the environment and events are become more needed and important.

As a result of all mentioned above, we calculated the reaction cross–sections of ^{9}Be and ^{16}O using TALYS 1.6 [4] and EMPIRE 3.2 [5, 6] codes for (n, α), (n, 2n), (n, t), (n, El) and (n, TOT) reactions. In addition, by using Geant4 [7] the total reaction cross section for BeO composite material was calculated since it is not possible to perform the composite material computations with neither TALYS 1.6 nor EMPIRE 3.2. Also with Geant4 code, the generated isotopes and particles were obtained for a situation in which BeO is used as a neutron moderator. Results have been correlated with each other and also against the Experimental Nuclear Reaction Data Library, EXFOR [8].

2. Calculation Methods

Two versions of the exciton model, which are Two Exciton model in TALYS 1.6 and Exciton model in EMPIRE 3.2 computer software, were used for the reaction cross section computations of ^{9}Be and ^{16}O target nuclei.

In the Two–Component Exciton model, which is the default model for TALYS reaction cross section computations, the particles and holes are followed throughout the reaction. The notation for the following equation gives the numbers of particles – which could be proton or neutron – and holes as $p_\pi(p_\nu)$ and $h_\pi(h_\nu)$, respectively. From this, the proton exciton number is defined as $n_\pi = p_\pi + h_\pi$ and the neutron exciton number as $n_\upsilon = p_\upsilon + h_\upsilon$ which give us to construct the charge independent particle number as $p = p_\pi + p_\upsilon$, the hole number as $h = h_\pi + h_\upsilon$ and the exciton number as $n = n_\pi + n_\upsilon$.

Cross section σ^{CF}, and an emission rate W_k are given in Eq 1.

$$\frac{d\sigma_k^{PE}}{dE_k} = \sigma^{CF} \sum_{p_\pi=p_\pi^0}^{p_\pi^{max}} \sum_{p_\nu=p_\nu^0}^{p_\nu^{max}} W_k(p_\pi, h_\pi, p_\nu, h_\nu, E_k)\tau(p_\pi, h_\pi, p_\nu, h_\nu) \times P(p_\pi, h_\pi, p_\nu, h_\nu) \quad (1)$$

The compound formation cross section σ^{CF}, which is given by

$$\sigma^{CF} = \sigma_{reac} - \sigma_{direct} \quad (2)$$

is the basic feeding term for pre–equilibrium emission. In here σ_{reac} is directly obtained from the optical model and σ_{direct} is the sum of the cross sections for direct reactions to discrete states $\sigma^{disc,direct}$ as defined in Eq. (3) [4].

$$\sigma^{disc,direct} = \sum_i \sum_{k=n,p,d,t,h,\alpha} \sigma_{n,k}^{i,direct} \quad (3)$$

EMPIRE uses the Exciton [9] model PCROSS module for reaction cross section computations of pre–equilibrium reactions. A unified model is used by the exciton model that is the solution of a key equation that previously represented by Cline [10] and Ribansky [11].

Beside the theoretical reaction cross section computations of ^{9}Be and ^{16}O nuclei for different neutron induced reactions with TALYS 1.6 and EMPIRE 3.2, in this study; Geant4 which is simulation and computation software, used to simulate hadronic interactions and calculate the reaction total cross–section for BeO in neutron induced reaction simulation. Geant4 is an open source program which is created and distributed by the Geant4 collaboration [12]. There exists many models available in Geant4 inside itself for different type of simulations and computations for various physical events.

To serve the purpose of this study, G4HPmodel (High Precision) was used which a data is driven model and covers up to 20 MeV from the thermal energies. In this model; for elastic process NeutronHPElastic, for inelastic process NeutronHPInelastic and for capture process NeutronHPCapture libraries were used [13]. In our case, the aim of that models usage was to simulate the interaction of neutrons with a BeO sphere of radius 30 cm that located in the vacuum structure. Our computations were repeated with 1000 runs including 10000 neutron particles for each run. In the center of BeO sample, 14.1 MeV neutrons created and flight randomly. By running Geant4 for studied case, we simulated the number of neutrons passed through the material also the generated isotopes and particles due to the hadronic interactions. In the second part of Geant4 usage, we calculated the total reaction cross–section for (n,TOT) reaction with 0-15 MeV energetic incident neutron particles in BeO sample.

3. Results and Discussions

In this research, reaction cross sections of $^{9}Be(n,2n)^{8}Be$, $^{9}Be(n,\alpha)^{6}He$, $^{9}Be(n,t)^{7}Li$, $^{9}Be(n,EL)$, $^{9}Be(n,TOT)$ and $^{16}O(n,2n)^{15}O$, $^{16}O(n,\alpha)^{13}C$, $^{16}O(n,t)^{14}N$, $^{16}O(n,EL)$, $^{16}O(n,TOT)$ have been calculated for Two Component Exciton and Exciton models with TALYS 1.6 and EMPIRE 3.2 codes. Results are given in Figs. 1–5. Experimental data shown in the figures are taken from EXFOR.

The calculated cross sections of $^{9}Be(n,2n)^{8}Be$ and $^{16}O(n,2n)^{15}O$ reactions have been given with the experimental data in Fig. 1 (a) and (b), respectively.

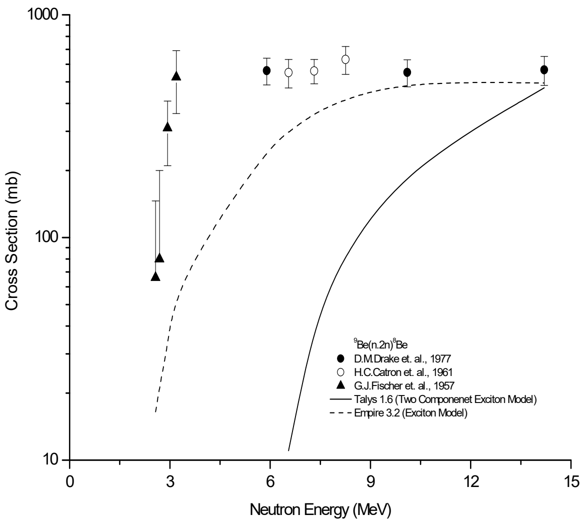

Figure 1 (a). The $^{9}Be(n,2n)^{8}Be$ reaction computation with EXFOR experimental data.

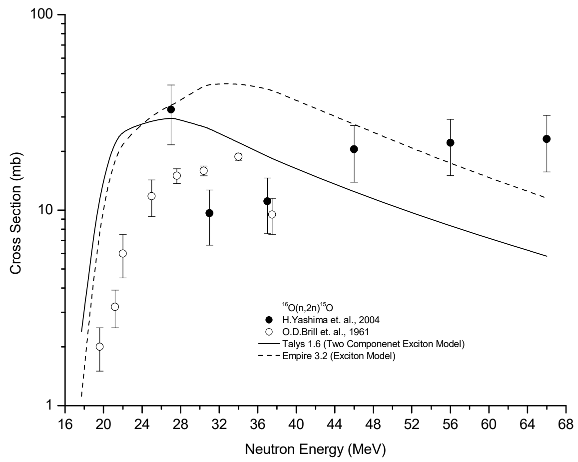

Figure 1 (b). The $^{16}O(n,2n)^{15}O$ reaction computation with EXFOR experimental data.

The TALYS 1.6 Two Component Exciton and EMPIRE 3.2 Exciton computation results are below the experimental data to 15 MeV in Fig. 1 (a). For Fig. 1 (b), calculated results are in consensus with the experimental results but they pursue experimental data from above in the neutron energy region of 16-25 MeV and EMPIRE 3.2 Exciton model computations are in agreement with the experimental results including error strips in the neutron energy region of 45-57 MeV.

The comparison of calculated cross–sections of $^{9}Be(n,\alpha)^{6}He$ and $^{16}O(n,\alpha)^{13}C$ reactions with the experimental values given in Fig. 2 (a) and (b), respectively.

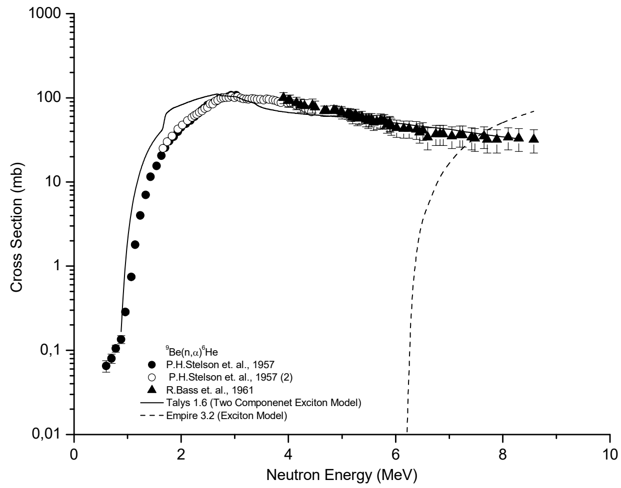

Figure 2 (a). The $^{9}Be(n,\alpha)^{6}He$ reaction computation with EXFOR experimental data.

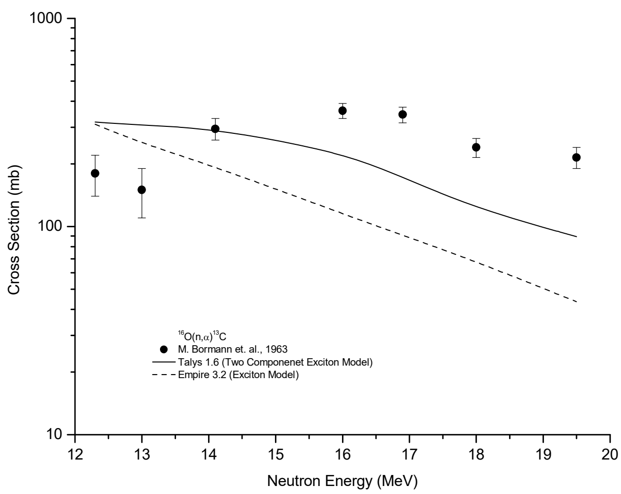

Figure 2 (b). The $^{16}O(n,\alpha)^{13}C$ reaction computation with EXFOR experimental data.

TALYS 1.6 Two Component Exciton model computations for $^{9}Be(n,\alpha)^{6}He$ reaction are almost the same with the experimental results. Also for $^{16}O(n,\alpha)^{13}C$, model computations give lover results than the EXFOR data in the neutron energy region of 14,5-20 MeV.

The experimental and theoretical results of $^{9}Be(n,t)^{7}Li$ and $^{16}O(n,t)^{14}N$ reactions have been given in Fig. 3 (a) and (b).

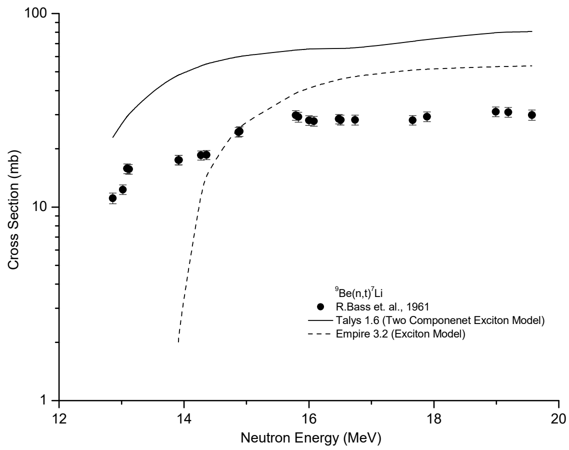

Figure 3 (a). The ^{9}Be(n,t)^{7}Li reaction computation with EXFOR experimental data.

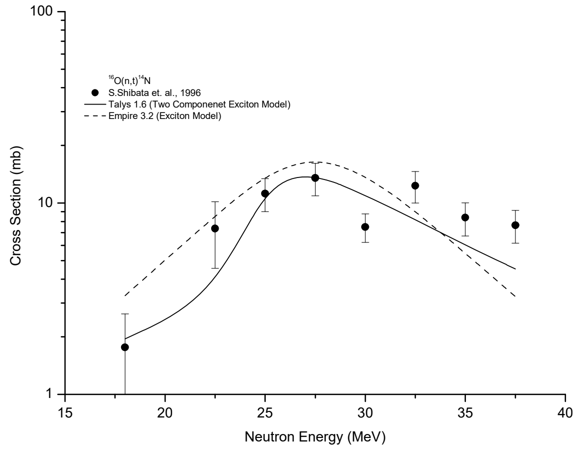

Figure 3 (b). The ^{16}O(n,t)^{14}N reaction computation with EXFOR experimental data.

^{9}Be(n,t)^{7}Li reaction cross section results of the TALYS 1.6 Two Component Exciton model are above the experimental values and EMPIRE 3.2 Exciton model follow the experimental data from above in the energy region of 14,5-20 MeV. The calculated cross sections for ^{16}O(n,t)^{14}N reaction with the experimental values are given in Fig. 3 (b). Both model computations are in agreement with the experimental results up to 30 MeV neutron incident energy. After this energy, they show a little discrepancy with the experimental data.

The comparison of neutron induced elastic reaction cross sections computations for ^{9}Be and ^{16}O are also performed and given in Fig. 4 (a) and (b). In this figures, J. B. Marion et al. [14] and M. Sugimoto et al. [15]'s experimental results are shown with EMPIRE 3.2 Exciton model computations in agreement up to 7 MeV incident neutron energy. However, more than 7 MeV energies all model computations shows disagreement for ^{9}Be(n,EL). For the studied energy range; Two Component Exciton model of TALYS 1.6 and Exciton model of EMPIRE 3.2 give similar results and both are in good agreement with the experimental results for ^{16}O(n,EL) reaction.

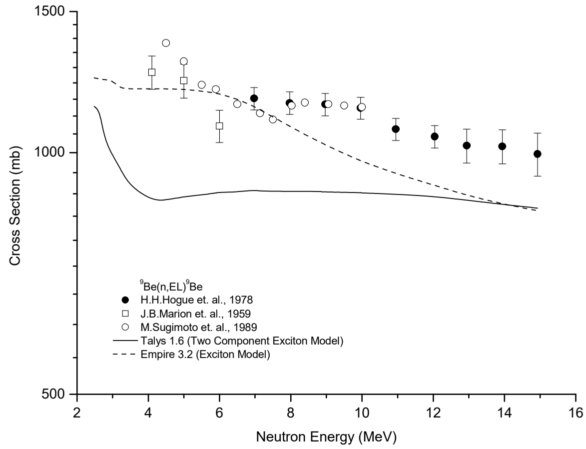

Figure 4 (a). The ^{9}Be(n,EL) reaction computation with EXFOR experimental data.

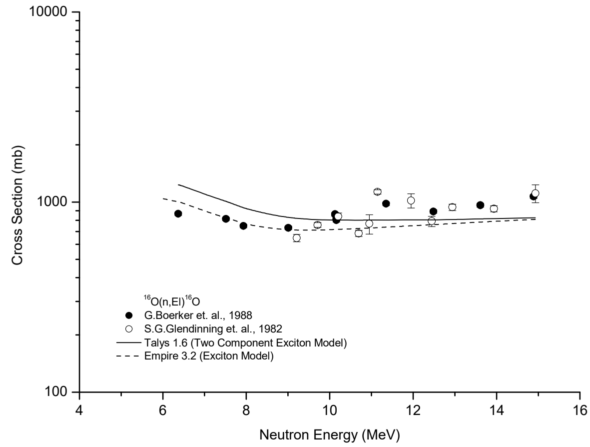

Figure 4 (b). The ^{16}O(n,EL) reaction computation with EXFOR experimental data.

Beside all of the computations mentioned above, neutron induced total reaction cross section computations for ^{9}Be, ^{16}O and BeO composite materials have been studied. Comparisons of that results given in Fig. 5 (a), (b) and (c), respectively.

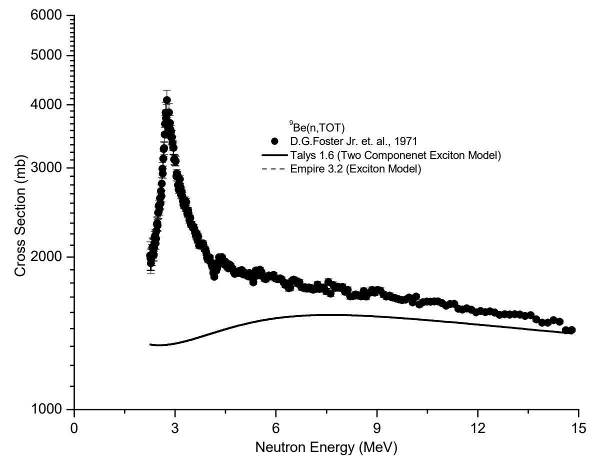

Figure 5 (a). The ^{9}Be(n,TOT) reaction computation with EXFOR experimental data.

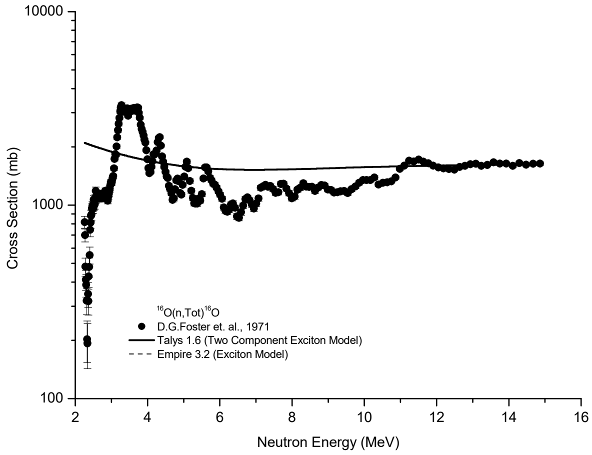

Figure 5 (b). The ^{16}O(n,TOT) reaction computation with EXFOR experimental data.

EMPIRE 3.2 and TALYS 1.6 model computations give almost the same results with each other for both ^{9}Be(n,TOT) and ^{16}O(n,TOT). Due to that, in Fig. 5 (a) and (b) it is not clearly visible that EMPIRE 3.2 and TALYS 1.6 results. On the other hand, both models disagree with the experimental results for lover than 11 MeV energy range but greater than this energy, computation model results became convenient.

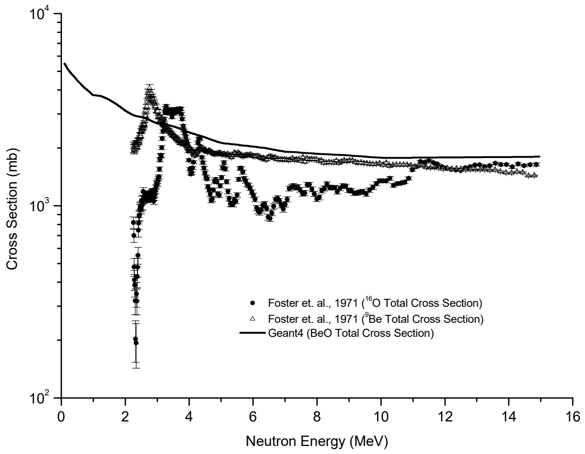

Figure 5 (c). The BeO(n,TOT) reaction computation with EXFOR experimental data.

In Fig. 5 (c), BeO(n,TOT) reaction total cross section computations by using Geant4 compared with Foster and Glasgow[16]'s experimental results for ^{9}Be and ^{16}O. As it shown from the Fig. 5 (c), calculated values form Geant4 for BeO are greater than experimental values of ^{9}Be and ^{16}O total cross section values after 4 MeV incident neutron energy. The results are closer to ^{9}Be experimental values between the energy ranges of 4 – 16 MeV. The reason of that is the ^{9}Be density in BeO, which is greater than ^{16}O.

Simulation studies with Geant4 give us the list of generated isotopes and secondary particles due to the hadronic interactions of BeO moderation material with incident neutrons. The list is presented in Table 2.

Table 2. The list of generated particles and their properties

Particle	Mean Number	E_{mean} (MeV)	E_{min} --> E_{max}
^{9}Be	63	0,94715	7.5381 keV --> 4.7725 MeV
^{12}C	9	1,3505	226.56 keV --> 2.8257 MeV
^{13}C	13	2,1602	345.46 keV --> 4.3164 MeV
^{7}Li	2	1,6523	1.5831 MeV --> 1.7216 MeV
^{15}N	1	0,1769	176.9 keV --> 176.9 keV
^{16}N	4	1,1644	395.67 keV --> 1.7872 MeV
^{16}O	86	0,7938	7.8703 keV --> 3.136 MeV
Alpha	92	3,3498	94.369 keV --> 17.334 MeV
Deuteron	1	4,0285	4.0285 MeV --> 4.0285 MeV
Gamma	169	1,9482	1.14 keV --> 7.1152 MeV
Neutron	103	3,563	173.08 keV --> 11.427 MeV
Proton	4	2,486	1.0935 MeV --> 3.7774 MeV
Triton	2	2,782	1.3649 MeV --> 4.1992 MeV

Also, energy deposition along BeO material show in Fig. 6. More energetic particles flight more so could travel more and reach to end of the material. BeO material sample has a radius of 30 cm and less amount of more energetic particles could reach to the end. Due to that, a decrease occurs in the graph systematically.

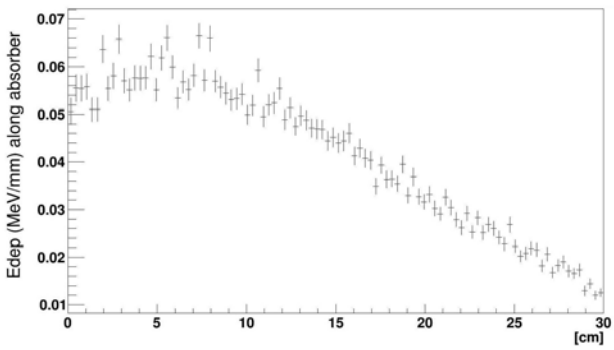

Figure 6. Energy deposition (MeV/mm) in BeO for 0 to 30 cm using Geant4 code.

4. Summary and Conclusions

In this study, the reaction cross sections of (n,α), (n,2n), (n,t), (n,EL) and (n,TOT) reactions for ^{9}Be and ^{16}O isotopes have been calculated by using the TALYS 1.6 and EMPIRE 3.2 computation codes. The theoretical computation results have been compared with the experimental data taken from the EXFOR database. Also, hadronic interactions were investigated and generated isotopes–particles were obtained for BeO as a neutron moderator by using GEANT4. In addition, energy deposition along BeO material was obtained. The results can be given as following:

1. The TALYS 1.6 Two Component Exciton model computations give similar results only with experimental values for $^{9}Be(n,\alpha)^{6}He$. On the other hand EMPIRE 3.2 Exciton model computations are the best for ^{16}O(n,EL) reaction.

2. For (n,TOT) reaction cross section computations with TALYS 1.6 and EMPIRE 3.2 models for both ^{9}Be and ^{16}O gives the same results almost.

3. Due to the hadronic interactions occurred in BeO, generated secondary particles and isotopes have been investigated and given in Table 2. For 14.1 MeV induced neutron interactions, energy range between 173.08 keV and 11.427 MeV neutrons with average energy of 3.563 MeV have been observed. This situation shows us that BeO reduces the energy of incoming neutrons and produces low energetic less amount of neutrons.

4. Energy deposition along the absorber material BeO has been investigated. Less amount of more energetic particles could reach to the limit of sample size. Due to that, a decrease occurs in the graph of E_{dep} versus sample length systematically. This property of the material give us the ability of usage as a good neutron moderator material.

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