

Comparative Analysis of the Excitation Functions of ^{238}U as Breeder Fuel Using OPTMAN Code.

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Abstract

The comparative analysis of the excitation function of Uranium-238 was carried out using a Coupled-Channelled Optical Model code, OPTMAN. The high demand for nuclear reactor fuels has necessitated this research. As one of the major naturally occurring radioisotope of Uranium with lots of fuel prospect, Uranium-238 occur in large quantities (99%). Two steps process away from Uranium-238 on neutron capture can produce fissile materials to be used as reactor fuel. Though, Uranium-238 is not by itself a fissile material. But, it is a breeder reactor fuel. Computations were done for both the Potential Expanded by Derivatives (PED) which account for the Rigid-Rotor Model (RRM) that treat nuclei as rigid vibrating sphere as well as account for nuclear volume conservation and Rotational Model Potentials (RMP) which account for the Soft-Rotator Model (SRM) that treat nuclei as soft rotating spherical deformed shapes. Each of the calculated data was compared with the retrieved data from Evaluated Nuclear Data File (ENDF) which was found to be in good agreement. The threshold energies in all cases were found to be 4 MeV for both PED (Potential Expanded by Derivatives) and RMP (Rotational Model Potentials). It is observed that results from RMP much better agreed with the retrieved data than one obtained from PED.

1. Introduction:

Nuclear fission is almost ten (10) times much effective at energy of production compare to normal fossil (fuels) [1]. Nuclear reactions generate and produce massive quantities of carbon-free electricity and aside from this volume of energy produced, it protects the environment and the air we breathe [2]. In some developed countries, like U.S, Nuclear is one of

the biggest clean sources of power. Electricity of close to 800 billion kilowatts per hour is generated each year making more than one-second of the nation's electricity (emissions-free). Producing electricity is not the only use of nuclear reactors, as reactors can either be power reactors or research reactors. But, both reactors use radioactive materials as fuels. Majorly, Uranium is the best radioactive material that is readily available as fuel [3].

Uranium occurs in the earth's crust naturally and is gently radioactive in nature. It happens to be the only element that has naturally occurring fissile isotope [4]. However, due to the scarcity of Uranium-235 isotopes, Nuclear Physicists are making efforts to seek alternative fuels. Uranium is found

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in nature as Uranium-238 with about 99.2739 to 99.2752%, Uranium-235 with about 0.7198 to 0.7202% and lesser quantity of Uranium-234 with about 0.0050 to 0.0059% [5].

Therefore, to have enough nuclear fuel or reactor fuel, Uranium-238 is irradiated by a fast neutron to produce Uranium-239 and this Uranium-239 can undergo radioactive decay to produce Plutonium-239. Plutonium-239 just like Uranium-235 is a fissile material [6]. Plutonium-239 can therefore be battered with neutrons of high-speed. On absorption of these free neutrons, the nucleus of plutonium breaks in two fragments fission which latter deconfine heat and more neutrons and in turns splits other nuclei of plutonium, allowing still more other neutrons. Repetition of this process sustained chain reaction resulting to cheap and steady energy source transported from the core of the reactor through the coolant of liquid sodium to a system of heat exchange [7]. This system makes use of these heat in production of steam for the turbine to drives the generator of electric. Aside from Uranium-238 which can be irradiated to produce fissile material, other fertile materials can equally be irradiated to produce fuel materials for the reactors. Such materials like Thorium-232, Uranium-234, etc. are fissionable but fertile materials that can be used as fuel via two steps process [8].

It is more interesting that as the traditional nuclear reactor uses the fissionable but rare isotopic Uranium-235 only for fuel, but a breeder reactor uses either Uranium-238 or Thorium-232 in which only sizeable amount are available [9]. This shows that in breeders, close to 70% of the isotopes can be used to produce power. The two naturally occurring materials for fertile are Uranium-238 and Thorium/232 only [10].

Fissile materials also called fissionable materials are kind of nuclei that underwent the fission reaction. The basic materials for fissile are Uranium-235 with about 0.7% naturally occurrence, Plutonium-239 and Uranium-233. The last two have been produced artificially from material for fertile of Uranium-238 and Thorium-232 respectively [11]. This work investigates the effect of rotational excitation in neutron induced Thorium-Uranium actinide cycle of 20 MeV using Coupled-Channels Optical Model OPTMAN Code with adjustment for soft and rigid rotation of the nucleus.

2. Theory:

The current optical potential encompasses corrections (relativistic) as reported by Kawano (2020) [12], and expanded by Goriely et al (2019) [13].

Surface variation $W_D(E)$ and potential for volume absorption $W_V(E)$ can wisely be presented in terms of energy which could be suitable for the dispersive optical model analysis [12], [13]. The most utilized energy (dependence) for the surface (imaginary) term has been pointed out by Avrigeanu

& Avrigeanu, (2023) [14] as.

$$W_D(E) = A_D \left[\frac{(E - E_F)^{-2}}{(E - E_F)^{-2} + (B_D)^2} - \exp(-\lambda_D(E - E_F)) \right] \quad (1)$$

A_D , B_D and λ_D are constants (undetermined), E and E_f are Proton and fermi energy respectively.

Another utilized energy (dependence) for the surface (imaginary) term has been pointed out by Naik et al, (2021) [15] Naik et al, (2020) [16] as follow;

$$A_{D,V} = W_{D,V}^{DISP} \left[1 + (-1)Z' + 1 \frac{C_{wiso,wviso}N - Z}{W_{D,V}^{DISP} A} \right] \quad (2)$$

$W_{D,V}^{DISP}$ and $C_{wiso,wviso}$ are constants (undetermined), A , N and Z are mass, neutron and atomic number respectively.

Utilized energy (dependence) for the volume (imaginary) term has been confirmed in studies of nuclear matter theory by Brown and Rho (2021) [17]

$$W_V(E) = A_V \frac{(E - E_F)^2}{(E - E_F)^2 + (W_V^{DISP})^2} \quad (3)$$

A_V and W_V^{DISP} are constants (undetermined), E and E_f are proton and fermi energy respectively [18], [19], [20], [21], [22], [23] and [24].

3. Methodology:

The OPTMAN code for this work was downloaded from the IAEA website at <http://nds-IAEA.org>. The optical model code OPTMAN was chosen because it can study nucleon interactions with light-mass, medium-mass, and heavy-mass nuclei for a broad range of energy up to 200 MeV. Additionally, it has a Soft-Rotator model in addition to its Rigid-Rotator model, which improves the precision of the even-even nuclide.

The selection of the appropriate record cards and switches determines how the code will run when the software has been successfully installed using the G-FOTRAN compiler. Record cards that describe input data are themselves described by switches for the description of the model. The "va" executable file is used to invoke each calculation's input data and is produced using the Windows command The code is executed immediately the command "va" is issued, the input file name is requested and supplied, the output file name is requested and supplied, and the enter key is pushed. The OPTMAN code computation was based on Equation (1) to (3).

4. Results and Discussions:

The results obtained from the computer software (OPTMAN Code) based on the Equation (1) to (3) for Rotational

Model Potential (RMP) which accounts for Soft-Rotator Model and Potentially Expanded by Derivatives (PED) accounts for Rigid-Rotor Model by calculating the neutron-induced Total Potentially Expanded by Derivatives (TPED) and Total Rotational Model Potential (TRMP), Reaction Potentially Expanded by Derivatives (RPED) and Reaction Rotational Model Potential (RRMP) and Elastic Potentially Expanded by Derivatives (EPED) and Elastic Rotational Model Potential (ERMP) cross section reactions for ²³⁸U is presented in Table 1 below:

Table 1. Results Obtained for Soft and Rigid-Rotor Model.

Energy (MeV)	Cross Section (Reaction)			Cross Section (Elastic)			Cross Section (Total)		
	PED	RMP	ENDF	PED	RMP	ENDF	PED	RMP	ENDF
4.00	1.81	1.76	0.55	1.86	1.87	4.45	3.67	3.63	5.00
5.00	1.66	1.62	0.55	2.02	2.67	4.34	3.68	3.69	4.89
6.00	1.63	1.59	0.61	2.22	2.29	4.08	3.85	3.88	4.69
7.00	1.65	1.61	0.94	2.40	2.48	3.59	4.05	4.09	4.53
9.00	1.65	1.61	1.01	2.59	2.68	2.97	4.34	4.29	3.98
10.00	1.63	1.58	1.00	2.60	2.67	2.83	4.22	4.26	3.83
12.00	1.58	1.53	0.97	2.47	2.50	2.72	4.05	4.04	3.69
14.00	1.56	1.52	1.14	2.24	2.24	2.79	3.80	3.76	3.93
16.00	1.57	1.54	1.31	1.99	1.97	3.02	3.56	3.51	4.33
18.00	1.58	1.56	1.32	1.77	1.73	3.25	3.35	3.29	4.57
20.00	1.57	1.56	1.41	1.58	1.54	3.40	3.15	3.10	4.81

To compare the obtained results from this study with retrieved data (TENDF), charts for the computation of the excitation function for the cross-section (Total), cross-section (Reaction) and cross-section (Elastic) of ²³⁸U are plotted and presented in Figure 1, 2 and 3.

Based on Figure 1, the excitation function of the neutron-induced total cross section of ²³⁸U shows the same trend which increased from 4 – 9 MeV and decreased from 9-20 MeV. The result obtained from Total Rotational Model Potential (TRMP) agrees more with the retrieved data (TENDF) than the Total Potential Expanded by Derivatives (TPED). Furthermore, the effect of rotational excitation is more obvious and is best accounted for by Rotational Model Potential.

According to Figure 2, the excitation function of Uranium-238 shows agreement between both RPED and RRMP with the retrieved standard data (RENDF) from 4-6 MeV. This indicates threshold energy for the neutron-induced reaction for both Potential Expanded by Derivatives (RPED) and Rotational Model Potential (RRMP) to be ≤ 4 MeV.

Additionally, there is poor agreement between the calculated PED values with the standard data of ENDF from 6-12 MeV. Results from Rotational Model Potential show better agreement with the retrieved standard data (RENDF) than the Potential Expanded by Derivatives. This shows that the changing nature of the nucleus under rotation is best described by the Rotational Model Potential.

Figure 3 indicated that for the neutron-induced elastic scat-

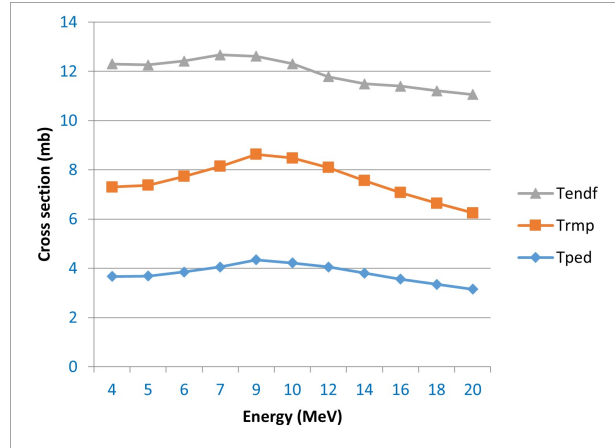


Figure 1. Concentrations of erythropoietin in serum of patients and healthy groups.

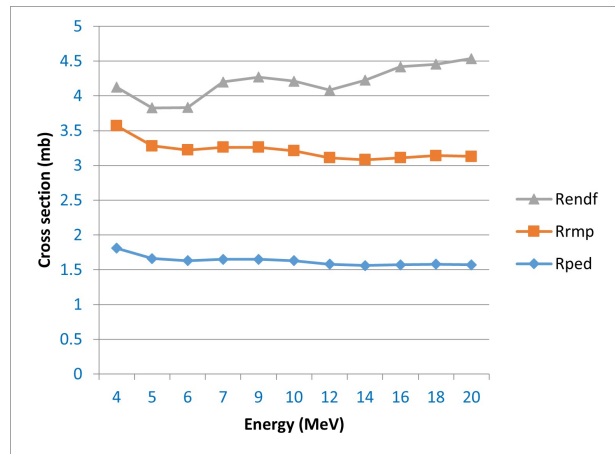


Figure 2. Reaction Cross Section of ²³⁸ U.

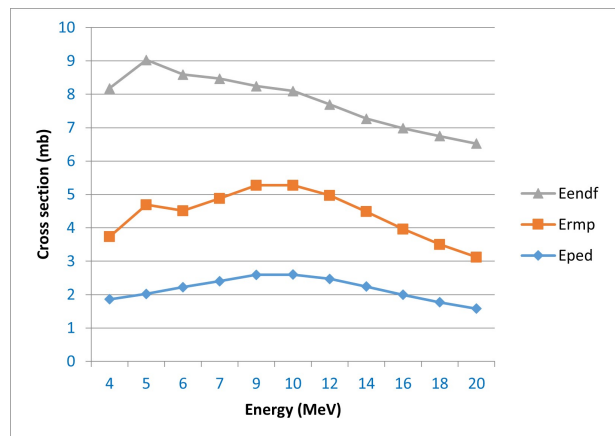


Figure 3. Elastic Cross Section of ²³⁸ U.

tering in both Potential Expanded by Derivatives (EPED) and the Rotational Model Potential (ERMP) there is an agreement with retrieved data (EENDF) observed between 4 to 6 MeV and 10 to 20 MeV. But no agreement between EPED and the retrieved EENDF standard data from the 6 to 9 MeV.

This, indicates that the Rotational model potential which accounts for the soft-Rotor model of the Coupled-channels Optical Model is best used to describe the effect of rotation under excitation on neutron capture and agreed more with the standard data (EENDF).

5. Conclusions:

A coupled-channel optical model OPTMAN code was used to investigate the effects of rotational excitation in neutron induced ^{238}U cycle actinide up to 20 MeV. Optical model computations were carried out via the OPTMAN code using the Coupled-Channel Rotational Model Potential (CC-RMP) which describe the Soft-Rotor model that treat nuclei as soft rotational sphere or deformed nuclei and Potential Expanded by Derivatives (CC-PED) which described Rigid-Rotor Model that treat nuclei as rigid vibrating sphere and account for nuclear volume conservation. From the computations performed for both PED and RMP, the energies agreed with the standard retrieved data (ENDF) are observed to be 4 MeV. It was revealed also that the results obtained from using Rotational Model Potential (RMP) are generally higher and are in better agreement with the standard ENDF data than those obtained from the Potential Expanded by Derivatives (PED).

However, results using both PED and RMP for elastic scattering cross sections are generally higher for ^{238}U and showed better agreement with the retrieved ENDF data. Furthermore, the Odd-A nuclides tend to have higher cross section values when compared with the Even-A nuclides. Since the oddness of both Z and N tends to lower the nuclear binding energy, making odd nuclei less stable and more likely to undergo fission, all odd-A nuclei used in this research could be best for reactor fuel, except for the fissionable but not fissile materials. It is therefore recommended that, the odd-A nuclei used in this work be tested as reactor fuel.

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Declarations:

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تحليل مقارنة لدالة استثارة ^{238}U كوقود للتوليد باستخدام كود *OPTMAN*

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الخلاصة

تم إجراء التحليل المقارن لدالة استثارة اليورانيوم 238- باستخدام كود النموذج البصري ذي القنوات المزدوجة *OPTMAN* ، استلزم الطلب الكبير على وقود المفاعلات النووية إجراء هذا البحث. يعتبر اليورانيوم 238- كواحد من النظائر المشعة الرئيسية لليورانيوم الطبيعي حيث يوجد اليورانيوم 238- بكميات كبيرة (99%) . يمكن أن ينتج النووي من خطوتين بعيداً عن اليورانيوم 238- عند التقاط المواد الانشطارية لنيوترونات. على الرغم من أن اليورانيوم 238- ليس في حد ذاته مادة انشطارية. لكنها وقود مفاعل مستولد. تم إجراء الحسابات لكل من المشتقات المحتملة الموسعة (*PED*) والتي تمثل نموذج الدوار الصلب (*RRM*) الذي يعامل النوى على أنها كرة اهتزازية صلبة بالإضافة إلى حساب الحفاظ على الحجم النووي وإمكانات النموذج الدوراني (*RMP*) التي تمثل نموذج دوار ناعم (*SRM*) يتعامل مع النوى كأشكال كروية مشوهة دوار ناعمة. تمت مقارنة كل من البيانات المحسوبة بالبيانات المسترجعة من ملف *Dada* النووي المقيم (*ENDF*) والذي وجد أنه في توافق جيد. تم العثور على طاقات العتبة في جميع الحالات لتكون $\geq 4\text{MeV}$ لكل من *PED* . ويلاحظ أن نتائج *RMP* تتفق بشكل أفضل مع بيانات *ENDF* من تلك التي تم الحصول عليها من *PED* .

الكلمات الدالة : وقود مفاعل استنسال؛ كود *OPTMAN* ؛ نموذج بصري مزدوج القنوات ؛ نموذج الدوار الصلب (*RRM*) ؛ الموسعة المحتملة بواسطة المشتقات (*PED*) .

التمويل : لا يوجد.

بيان توفر البيانات: جميع البيانات الداعمة لنتائج الدراسة المقدمة يمكن طلبها من المؤلف المسؤول.

اقرارات:

تضارب المصالح: يقر المؤلفون أنه ليس لديهم تضارب في المصالح.

الموافقة الأخلاقية: لم يتم نشر المخطوطة أو تقديمها لمجلة أخرى، كما أنها ليست قيد المراجعة.