Influence of different data tables on neutron induced reactions in quasi-infinite $^{238}\text{U}$ and $^{232}\text{Th}$ targets irradiated by protons with relativistic energy

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Abstract. The last decade saw the emergence of various theoretical analysis and developments of ADS (Accelerator Driving System). Different transport codes, nuclear models and nuclear cross sections have been used to predict and estimate the properties of ADS. The energy of the proton beam is supposed to range between 1 and 1.5 GeV, but some analyses suggest higher energy – up to 10 GeV. The recent papers examine the influence of the nuclear models on neutron induced reactions (n,f), (n,g), (n,xn), (n,el.) and (n,inel.). The experimental set-ups and the presumable ADS constructions consist of thousands of segments and details for example project Myrrha, Belgium [1]. The calculation of the above reactions depends on the neutron spectrum in each segment. There is a considerable difference in the size of these segments in ADS, which makes the estimation of the influence of the nuclear models and the cross sections on the integral number of neutron induced reactions more difficult. This article considers the influence of different cross section data tables on neutron induced reactions in $^{238}\text{U}$ or $^{232}\text{Th}$ targets. One nuclear model describing the high energy part of the nuclear interaction and various cross section data tagle (ENDF, ENDL, TENDL2014 and etc.) are used. All particles generated in the nuclear interaction process deposit their energy in the target volume. MCNP 6.1 transport code was used.

1. Introduction

Introduction: In the last two decades the study of the possibilities for nuclear waste transmutation, as well as the use of $^{238}\text{U}$ and $^{232}\text{Th}$ for energy production in ADS, have received considerable attention. The ADS consists of three components: 1) target comprised of heavy metals such as lead, bismuth, tungsten, fissionable nuclides or a composition of the above metals; 2) reactor part comprised of high-enriched nuclear fuel (25-30% mix of $^{238}\text{U}$ and $^{239}\text{Pu}$) plus a cooling system; 3) proton accelerator 1-10 GeV. When the high-energy protons irradiate the target, high-energy particles are generated - neutrons, pions, protons, etc. The interaction of the high-energy particles with the uranium and thorium nuclei is described by nuclear models such as INCL4, QGSM, ISABEL, CEM, etc. All possible nuclear reaction channels are included in the models. These models are part of various transport codes such as MCNP6.1, FLUKA, GEANT4, MARS15, etc., which also include nuclear cross sections. Some of the transport codes have own neutron cross sections (neutron energy groups) like FLUKA, MCNP6.1 provides the opportunity to select cross sections for each nuclide. The standard tables of neutron induced cross reactions are defined for neutron energy up to 20 MeV or less. In MCNPX transport code it is possible to select cross sections for $^{238}\text{U}$ and $^{232}\text{Th}$ ranging between 20 and 200 MeV. The nuclear models in this transport code start when there are no cross sections. When we change only the nuclear cross sections in the input file, we can estimate their influence on the total number of fissions, captures and (n,xn) reactions. Up to now no experiments with ADS prototypes or a big target with neutron leakage less than
20% have been carried out. In order to provide a better comparison of the neutron induced reactions, we choose an infinite uranium/thorium target-sphere with a radius of 2 m. The proton source $E_p=4$ GeV ($4\pi$ geometry) is located in the center of the sphere. With this geometry the particle leakage from the sphere is negligible.

1. Simulations

This paper aims to demonstrate the influence of the cross section data tables on the total number of fissions, captures and $(n,xn)$ reactions in quasi–infinite $^{238}$U and $^{232}$Th targets. This means that all particles which participated in the interaction deliver their energy in the target volume and the particles leakage is negligible. We use $^{238}$U and $^{232}$Th spheres with $R=2$m and point proton source, $E_p=4$ GeV located in the centre of the sphere. The nuclear model which we use is INCL4 and the evaporation part is ABLA which are included in MCNP6.1 transport code. The cross sections data tables used in the calculations are shown in table 1 and 2. The features of the MCNP6.1 output file are extremely important. First: The number of $(n,f)$, $(n,\gamma)$ and $(n,xn)$ reactions are calculated with data table cross sections only. It is important to note that nuclear models calculate all type of neutron induced reactions, but these reactions are not involved in neutron particle balance. Second: charged particle-and gamma-induced fissions are not involved in the output file, but they are calculated by the program.

1.1 Calculations of the total number $(n,f)$, $(p,f)$, $(\pi,f)$, $(\gamma,f)$, $(n,\gamma)$ and $(n,xn)$ reactions

We can calculate the above reactions in three different ways. First: in the MCNP6.1 output file the total balance of all particles and the integral number of the nuclear reactions per one projectile are given, but charged particle- and gamma-induced fission are not included. Second: by the FM card which gives the number of reactions in a volume/cell per one projectile. The reactions are calculated by eq. 1:

$$C \int F_i(E) \sigma_i dE$$

where $F$ (number of particles/cm$^2$) is flux and $\sigma$ (1/cm$^2$) is cross section, $C$ is normalization constant. The equation (1) is defined only for cross sections data tables if they are available. If there are no cross sections data tables, MCNP uses nuclear models. All nuclear reaction channels are included in the models, but it is not possible to see them in the output file. The limitations of the neutron cross sections are published in the MCNP6.1 manual. These two methods are limited and cannot calculate reactions $(p,f)$, $(\pi,f)$, $(\gamma,f)$. Third: calculation of the energy spectra for all particles of interest with the F4 card measured in particles/cm$^2$. The number of the reactions can be calculated by eq. 2.

$$\sum F_i(E)\sigma_i(E)$$

Where $F_i(E)$ is a particle flux [particles/cm$^2$] for specific energy interval and $\sigma_i$ is the average cross section for the same energy bin. There are experimental measurements of $(n,f)$ cross sections for $^{238}$U and $^{232}$Th for incident neutron energy up to 200 MeV presented in [2], which can be used in eq. 2. By eq. (2) the total number of all reactions can be calculated.

2. Results and conclusions

The outcomes are shown in tables 1 and 2. The first column presents the maximum incident neutron energy, i.e. the energy limit of the neutron cross sections. The second column shows the total number of neutrons generated in the target-sphere. The third column presents the number of spallation neutrons with energy greater than that in column 1. Columns 4, 5 and 6 show the number of reactions occurring in the target-sphere calculated by MCNP6.1, eq. (1). If we want to calculate the total fission reactions, the eq. (2) has to be used for all particle-induced fissions. It is important to note that the neutron
multiplicity (the number of neutrons irradiated per one fission) depends on the energy of the incident particles [4,5]. If the neutron fission cross section is extended, then the neutron multiplicity must also be extended to the same energy.

**Table 1. Neutron-induced reactions in a big $^{238}$U sphere (R=2m), $E_p=4$GeV**

| Data table       | E (MeV) | $N_{total}$ | $N_{pall}$ | (n,xn) | (n,$\gamma$) | (n,f) |
|------------------|---------|-------------|------------|--------|--------------|-------|
| endf66d          | 20      | 556         | 200        | 12     | 338          | 60    |
| endl92(LLNL)     | 30      | 540         | 206        | 14     | 342          | 66    |
| endf70j          | 30      | 537         | 206        | 14     | 325          | 55    |
| t16-2003 (LANL)  | 30      | 508         | 205        | 14     | 325          | 55    |
| 100xs(LANL)      | 100     | 491         | 124        | 30     | 318          | 56    |
| TENDL2012        | 20      | 490         | 197        | 14     | 313          | 53    |
| TENDL2014        | 200     | 415         | 90         | 20     | 270          | 54    |

MCNP 2.7 was used only with TENDL2012/14 data tables calculations and INCL4/ABLA nuclear models. MCNP6.1 was used with all other cross sections plus INCL4/ABLA.

**Table 2. Neutron-induced reactions in a big $^{232}$Th sphere (R=2m), $E_p=4$GeV**

| Data table | E (MeV) | $N_{total}$ | $N_{pall}$ | (n,xn) | (n,$\gamma$) | (n,f) |
|------------|---------|-------------|------------|--------|--------------|-------|
| uresa      | 20      | 340         | 206        | 15     | 218          | 10    |
| endf66c    | 20      | 340         | 206        | 14     | 218          | 10    |
| endl92     | 30      | 323         | 188        | 16     | 211          | 11    |
| endf70c    | 60      | 332         | 147        | 23     | 223          | 13    |
| TENDL2012  | 200     | 355         | 87         | 39     | 236          | 18    |
| TENDL2014  | 200     | 354         | 87         | 38     | 236          | 19    |

In fact, the results received by MCNP6.1 for $^{232}$Th target with TENDL2012 and TENDL2014 [3] cross sections coincide. On the other hand, the same data table comparison for $^{238}$U shows significant differences for the reaction (n,xn) - 30%, the (n,$\gamma$) reaction and the total neutron production have a difference of 15% and the (n,f) reactions are the same which is an unexpected result. Besides, there is a difference of 17-18% in the (n,f) $^{238}$U reaction calculated with endl92 and endf70j. All other reactions and parameters for both data tables almost coincide. The analysis of 100xs (defined up to 100MeV) and endf70j (defined up to 30MeV) also shows a significant difference in the (n,xn) reactions - two times, but the reactions (n,f) coincide.

The (n,f) $^{232}$Th cross sections TENDL2014 and ENDF70 in the 0-60 MeV energy range coincide. In the energy range from 60 to 200 MeV the (n,f) $^{232}$Th cross sections decrease monotonically from 0.75 to 0.06 barns, but the experimental cross sections [2] are a plateau of 0.8 barns and are used in eq. 2. Despite the increase of the (n,f) $^{232}$Th experimental cross sections in comparison with TENDL2014 the total number of (n,f) $^{232}$Th reactions is lower (15%) than the one calculated by TENDL2014 in the energy range 0-200MeV. The cross sections of (n,xn)$^{232}$Th for TENDL2014 and ENDF70 in the energy range 1-30 MeV they actually coincide, but the total number of the reactions (n,xn) $^{232}$Th differs with 40%. Calculations shows that the neutron flux in $^{232}$Th target for the energy range from 1 to 200 MeV calculated with TENDL2014 is 30% higher than with ENDF70. It is the reason why the (n,f) and (nxn) reactions for $^{232}$Th are 30% more with TENDL2014 calculations than with ENDF70. For $^{238}$U target and ENDF92 and ENDF70 such difference in the neutron flux was observed.

The (n,$\gamma$) $^{238}$U cross sections are well-known TENDL2014 and ENDF70 coincide but the total number of captures in the $^{238}$U target fluctuates with 25% for different data tables. The difference is quite

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significant, because \((n,\gamma)^{238}\text{U}\) means \(^{239}\text{Pu}\) accumulation in the target. In contrast to the \((n,\gamma)^{232}\text{Th}\) reaction the fluctuation is 5%, which is much more acceptable. We should bear in mind that the \((n,\gamma)^{232}\text{Th}\) reaction means \(^{233}\text{U}\) accumulation in the target. The fluctuation of the total neutron production as a function of data tables for \(^{238}\text{U}\) and \(^{232}\text{Th}\) targets is 30% and 5% respectively. All these calculations of neutron-induced reactions in the massive target or ADS based on \(^{238}\text{U}\) and \(^{232}\text{Th}\) show that the data cross sections are important. If the neutron-induced reactions are calculated in relatively small cells or regions in the targets/ADS, the above results are not visible and the calculations are within the error range.

3. References

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