A STUDY OF ACCELERATOR DRIVEN SUB CRITICAL SYSTEM - MATERIAL USING THE CASCADE CODE

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In the existing situation of experimental data required for design and modeling of ADS and similar other applications, development and benchmarking of the simulation codes for providing reliable data has become essential. Amongst the intra nuclear cascade codes, CASCADE code which has been validated for the neutron production in proton collision with the high Z materials in the past, has been used to study nuclear behavior of some of the prominent ADS materials like, Th, U, Pb, Bi, W, Fe, Cr and Al in respect of reaction and production cross sections of isotopes and neutrons in a wide range of energy, 11 MeV to several GeV. Emphasis has been laid on the data of cross sections of (n, xn) reactions. It is found that their role is definite and effective in deciding fuel combinations. The code provides neutron cross section data which shows agreement with the existing experimental data and stresses need of further validation using precision data from the accelerators.

1. INTRODUCTION

With the availability of spallation neutrons the field of nuclear science has once again seen a spurt because of the possibility that measurement of neutron cross sections at higher than 20 MeV energy may be done with high accuracy. Such data is highly demanded in design and modeling of Accelerator Driven Sub critical Systems (ADS), beam therapy, shielding etc. and to fulfill the need of data to verify nuclear models to advance the work of simulation codes. Secondly, spallation source being capable in copious yield of neutrons is required in studies related to cold and ultra cold neutrons. As mentioned, during the last two decades enormous effort has been put in developing various simulation codes which generally encompass a big part of already developed fundamental nuclear and particle models and they are expected to be highly useful in providing nuclear data for design and modeling of nuclear devices such as ADS with comparatively lesser efforts and time required in conducting experiments. In this paper we focus attention on one simulation code, CASCADE code. For general features of many such simulation codes of transport of nuclear radiation through heterogeneous matter one is advised to see reference [1]. The CASCADE code is based on the intra nuclear cascade model of particle+nucleus collision developed at JINR, Dubna by Barashenkov and Toneev [2] and their compilation of nuclear reaction data. In fact, the compilation has worked like a school of thought to a series of developments for example Gudima, Mashnik and Toneev [3] developed a version of the model in the form of MARIAG code which later on modified to Cascade Excitation Model (CEM-95) by Mashnik [4] to give neutron multiplicity, single and double differential spectra up to He⁴ and pions and fission yield not only in case of proton interactions but even projectiles like neutron and pions. Barashenkov, Shubin, Konobeyev and Lunev in the year 1985 [5] made an integrated effort for the extension of the code up to TeV energy of particle transport in any material and named it as the Dubna CASCADE code. Average multiplicities of all particles and light nuclei and their angular as well as energy spectra are estimated directly by the code. After including the evaluated and parameterized data libraries for estimation of cross sections and the modular structure in the code [6, 7] the code was published by Barashenkov [8]. This version of the code was used for validation of the neutron yield [9, 10].
Subsequently, fission and evaporation models used in the code were modified by Kumawat and Barashenkov [11] and recently estimation of internal flux and radiation dose are also introduced and tested by making measurements using the Am+Be kind of neutron source [12].

In this paper, we have presented results of simulation of physical quantities of fundamental interest such as neutron yield, production of various gases and isotopes by the CASCADE code in both proton and neutron collision with the nuclei of material useful for ADS and compared them as far as possible with the available experimental data. Emphasis is laid on the study of neutron growth by way of (n, xn) reactions at higher than reactor energies. Cross sections of some of the (n, xn) reactions being comparable to fission cross sections and the relationship between the (n, xn) and fission processes may affect the design of ADS as the heat distribution and growth of fission neutrons are affected. Efforts are made to present the data of the code in numerical or the graphical mode so that it may be used in the benchmark study of the codes.

2. REACTION CROSS SECTIONS

Most of the particle transport codes provide results of simulation in the form of fractions of events and they are converted to cross sections using the data of reaction cross sections. CASCADE code uses the phase shift analysis to estimate the reaction and elastic cross sections. In fact, repeatability of experimental data of reaction cross sections may be treated as a test of computation capability the code more to the case of neutron reaction cross sections where physics understanding of the process is some what barred by the non availability of precision data. Koning et al. [13] in a detailed study have emphasized collection of precise reaction cross section data from the point of design and development of ADS, study of fusion reactions and the optical model. In the following Fig. 1 CASCADE simulation data of non elastic reaction cross sections for transport of proton and neutron projectiles in $^{27}$Al have been plotted and compared with the available experimental data.

Data of p+$^{27}$Al reactions agrees nearly perfectly and in case of n+$^{27}$Al reaction cross sections small deviations at high energies may be because of the fact that the experimental data is from cosmic rays. This in turn emphasizes the need of precise accelerator data of neutron projectile at energy higher than 200 MeV. In Fig. 2 data of non elastic reaction cross sections of neutron with different target nuclei ranging from A=56 to 238 calculated from the CASCADE code and the optical model code [14] using Koning’s set of optical model

![Graph A](image1.png)

![Graph B](image2.png)

Fig.1. Comparison of reaction cross sections estimated from CASCADE code with the experimental data taken from the compilation [2]
parameters (OMP) in its library number 2405 [11] and described in references [15] and [16]. In the optical model calculations are possible up to 200 MeV and for the purpose of benchmark study of the CASCADE code we have presented results up to 1000 MeV. Results of CASCADE code are in agreement with the optical model in case of $^{56}$Fe and $^{232}$Th (OMP are available up to 50 MeV in case of $^{232}$Th) at all energies and small differences are noticed in case of $^{208}$Pb and $^{209}$Bi at energies ranging from 40-80 MeV.

One of the useful application of estimation of non elastic reaction cross sections of p+Al and n+Al has been made in solving the problem of non availability of experimental data of cross sections of monitor reactions of deuteron projectile, $^{27}$Al (d, 3p2n)$^{24}$Na at energies >200 MeV. In this energy range many accelerators that are producing deuteron beam, there is need of data of cross sections to monitor the beam flux by activation method. We have deduced [17] the production cross sections for the deuteron projectile using the principle of ‘factorization’ [18] and CASCADE data for the $^{27}$Al (p, 3pn)$^{24}$Na and $^{27}$Al (n, 2p2n)$^{24}$Na reactions. The deduced production cross sections of $^{27}$Al (d, 3p2n)$^{24}$Na reactions are plotted in Fig. 3 along with few experimental points. Here the fitted curve is for the CASCADE data. It may be seen that CASCADE data and the experimental points at $E_d = 2.33$ GeV [19] and at $E=6$ and 7.3 GeV [20] are in close agreement.

![Fig. 2. Non elastic cross sections from the optical model/RIPL [14] at energies 10-200 MeV for](image)

- $a$ - $^{56}$Fe
- $b$ - $^{208}$Pb
- $c$ - $^{209}$Bi
- $d$ - $^{232}$Th

$^{56}$Fe; $^{208}$Pb; $^{209}$Bi and $^{232}$Th are compared with that from the CASCADE code.
3. ISOTOPIC CROSS SECTIONS PRODUCTION

Beam window and target material in the ADS are irradiated to continuously to the beam of protons and the fuel material in the blanket by the produced neutrons give rise to different highly toxic and/or long lived isotopes and gases. Study of such isotopes and gases have attracted attention of experimentalists [21-24] from the point of providing data for design and modeling of ADS. In a paper all data of all materials can not be presented and we have selected few of them as representative cases. In Fig.4 production CS of $^{52}$Mn (half life 5.591d) in proton and neutron projectiles colliding with $^{56}$Fe material are plotted. In case of p+Fe collision Michel et al. [24] have presented similar data from different codes and experiments and qualitatively CASCADE data agrees reasonably well at E>50 MeV however, there is no experimental data available to compare in case of neutron projectile.

In Fig. 5 fractional yield of isotope production in CASCADE in case of 1 GeV p+$^{208}$Pb collision has been plotted and in table production CS of some isotopes of special interest like some gases and long lived ones are displayed. According to the CASCADE, 16.5 neutrons are produced in a thin Pb target in 1 GeV p+Pb collision for which the
fractional yield is presented then the cross section of $^4\text{He}$ - production per neutron is $555 \text{ mb}/16.5=33.64 \text{ mb/n}$ comparable to $\sim$35 mb/n of the experiment HINDAS [22] of Ta+p collision in the reverse kinetics. In column 3 of the table, $^4\text{He}$ production in 1 GeV n+Pb collision is also displayed but we understand that we need to perform simulations at different neutron energies to estimate average contribution of $^4\text{He}$ production by the secondary neutron flux colliding in the Pb target itself. Undoubtedly, total yield will be more than 555 mb as given here just for the proton colliding in thin target.

Production CS of some gases and long lived isotopes from the cascade code

<table>
<thead>
<tr>
<th>Product</th>
<th>p+Pb</th>
<th>n+Pb</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1\text{H}^2$</td>
<td>1.31 b</td>
<td>1.240 b</td>
</tr>
<tr>
<td>$^1\text{H}^3$</td>
<td>0.484 b</td>
<td>0.457b</td>
</tr>
<tr>
<td>$^3\text{He}^3$</td>
<td>0.053 b</td>
<td>0.049b</td>
</tr>
<tr>
<td>$^3\text{He}^4$</td>
<td>0.555 b</td>
<td>0.513b</td>
</tr>
<tr>
<td>$^{146}\text{Sm}<em>{62}$ ($T</em>{1/2}=10^8 \text{ y}$)</td>
<td>0.054 b</td>
<td>0.036</td>
</tr>
<tr>
<td>$^{151}\text{Sm}<em>{62}$ ($T</em>{1/2}=73 \text{ y}$)</td>
<td>0.006 b</td>
<td>-</td>
</tr>
<tr>
<td>$^{148}\text{Gd}<em>{64}$ ($T</em>{1/2}=74.6 \text{ y}$)</td>
<td>0.243 b</td>
<td>0.296</td>
</tr>
<tr>
<td>$^{150}\text{Gd}<em>{64}$ ($T</em>{1/2}=1.8\cdot10^6 \text{ y}$)</td>
<td>0.18 b</td>
<td>0.152</td>
</tr>
<tr>
<td>$^{154}\text{Dy}<em>{66}$ ($T</em>{1/2}=3\cdot10^6 \text{ y}$)</td>
<td>0.548 b</td>
<td>0.727</td>
</tr>
</tbody>
</table>

Fig. 5. Fractional isotopic yield in 1 GeV p$^{+208}\text{Pb}$ collision simulated in CASCADE

4. (n, xn) REACTIONS

So far there is very little experimental data is available for the (n, xn) reactions and it is understandable that they may play important role in a hybrid system. Secondly, this area of study combines the areas of isotopic and neutron yield in the environment of high energy neutrons. In this situation, we have simulated these reactions by CASCADE code in case of Bi$^{209}$ target and compared them with the experimental data of Kim et al. [25] in Fig. 6. The two data at x>3 are in agreement and both show existence of even-odd effect in Bi$^{209}$ [26].

In the following Fig. 7, CS are plotted for (n, xn) reactions with $^{52}\text{Cr}$ and $^{232}\text{Th}$ targets to show another evidence of the even-odd effect in even A nuclei as seen in case of odd A nucleus like Bi$^{209}$ in Fig. 6. Even-odd structures have been predicted in de-excitation code ABLA07 [26] in case of light particle emission in high energy nucleus + nucleus collision.

In the following Fig. 8 we have plotted cross sections of (n,xn) reactions with respect to xn neutrons produced in case of different energy neutrons with a) $^{91}\text{Zr}$ and b) $^{96}\text{Mo}$ and c) $^{181}\text{Ta}$ targets. It may be noted that with the increase of energy xn increases differently for different target masses and in case of high mass nuclei cross section of producing same number of neutrons (xn) is lower for higher energy. Average number of neutrons in pure (n, xn) for x=1,2,3… reactions, $<n(xn)>$ is compared with the total number of neutrons in the given reaction, $<n>$ in the form of the ratio, $<n(xn)>/<n>$ and plotted with the projectile energy in Fig. 9 for the three categories of materials i) light, ii) heavy but non fuel and iii) fuel nuclei of the ADS material.
Fig. 6. CASCADE data of cross sections of $^{209}$Bi(n, xn) reactions at: a) 32.8 MeV, b) 97 MeV, c) 132 MeV, and d) 147 MeV energy compared with experimental data by E. Kim et al. [25].

Fig. 7. Cross sections of (n, xn) reactions in even A nuclei: a) $^{52}$Cr and b) $^{232}$Th.

Fig. 8. Production cross section versus number of neutrons in (n, xn) reactions at energies ranging from 11 to 1000 MeV for: a) $^{91}$Zr, b) $^{98}$Mo, c) n+Ta$^{181}$. 
Fig. 8. Production cross section versus number of neutrons in \((n, xn)\) reactions at energies ranging from 11 to 1000 MeV for \(^{181}\text{Ta}\) (c)

The curves are drawn to guide the eyes. It can be pointed out that the percentage contribution of \((n, xn)\) reactions in case of fuel nuclei does not show any clubbing like that in the other two cases (where it is independent of the material of the category) and percentage contribution of \((n, xn)\) reactions at high energies decreases as \(^{233}\text{U} < ^{238}\text{U} < ^{232}\text{Th}\). Thus, Thorium is more prone to neutron multiplication by the \((n, xn)\) reaction and \(^{233}\text{U}\) is more fissionable. Although this fact needs experimental validation yet on its face it appears important from the point of settling down the question of combinations of fuel elements of ADS. It is expected that it will have noticeable effect on the heat distribution also. The detailed study of \((n, xn)\) reactions may prove important from the point of settling down the combinations of fuel elements for ADS and the heat distribution.

Fig. 9. Percentage contribution of \((n, xn)\) reactions in neutron production by different ADS material nuclei as function of neutron energy
5. DISCUSSIONS AND CONCLUSIONS

We have presented the CASCADE data for some selective nuclei and energy because of the limitations of space and in the readable graphical format for their comparison with other codes and experiments for the sake of benchmarking. It may be inferred that data of the reaction cross sections agrees with the experimental data as well as the models of fundamental interest such as optical model. Similarly, the data of production cross sections agrees well with the experiments. It may however be stressed that more precise neutron data is required to improve the code in case of reactions with neutron as a projectile. In respect of isotope data from the code there is need to introduce the concept of cumulative yield in the code so that its results may be compared with the experimental measurements.

From the present study of (n, xn) reactions the code results show presence of even-odd effect and other interesting results as in Fig. 9 which may help in selection of combinations of fuel elements for ADS logically. For both the cases, a more detailed study is required to be carried out from the simulation codes and experimentally with emphasis to the fuel elements.

For the study of effects of radiation damage, it may be mentioned that the present version of the code provides data of energy distributions of neutrons, protons and light charge particles such as d, t, \(^3\)He and \(^4\)He and it is not difficult to know such distributions of heavier secondary nuclei if required. However, presently the code gives average kinetic energies of all isotopes along with their production cross sections which is also useful for calculation of total radiation damage with the help of low energy codes like TRIM or IOTA. Efforts can be made to develop a unified code of high energy and low energy transport of all radiations produced in a beam transport in a medium.

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ИЗУЧЕНИЕ МАТЕРИАЛА СУБКРИТИЧЕСКОЙ СИСТЕМЫ, ВОЗБУЖДАЕМОЙ УСКОРИТЕЛЕМ, С ПОМОЩЬЮ ПРОГРАММ CASCADE

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При существующем положении дел с экспериментальными данными, требующимися для проектировки и моделирования ADS (accelerator driven systems) и для других аналогичных применений, становится важным разработка и эталонное тестирование программ modeling для обеспечения получения надежных данных. Из программ, существующих для внутриядерных каскадов, программа CASCADE, достоверность которой проверялась для рождения нейтронов при столкновениях протонов с материалами, имевшими в прошлом высокий атомный номер \( Z \), использовалась для изучения ядерного поведения некоторых известных материалов ADS (Th, U, Pb, Bi, W, Fe, Cr и Al) в отношении сечений реакций и сечений рождения изотопов и нейтронов в широком интервале энергий от 11 МэВ до нескольких гигаэлектронвольт. Особое внимание уделялось данным о сечениях реакций \( (n, xn) \). Найдено, что они играют определяющую роль при выборе сочетаний топлива. Программа дает данные о нейтронных сечениях, которые находятся в согласии с существующими экспериментальными данными, при этом подчеркивается необходимость дальнейшей проверки с использованием точных данных от ускорителей.

ВИВЧЕННЯ МАТЕРІАЛУ СУБКРИТИЧНОЇ СИСТЕМИ, ЩО ЗБУДЖУЄТЬСЯ ПРИСКОРОВАЧЕМ ЗА ДОПОМОГОЮ ПРОГРАММ CASCADE

В. Кумар, Х. Кумават, Читра Бхаттия

За існуючою стану справ з експериментальними даними, які необхідні для проектування та моделювання ADS (accelerator driven systems) і для інших аналогічних застосувань, важливими стануть розробка та еталонне тестування програм моделирования для забезпечення отримання надійних даних. Із програм, що існують для внутрішньоядерних каскадів, програма CASCADE, достовірність якої перевірялась для народження нейтронів при зіткненні протонів з матеріалами, що мали в минулому високий атомний номер \( Z \), використовувалась для вивчення ядерної поведінки деяких відомих матеріалів ADS (Th, U, Pb, Bi, W, Fe, Cr i Al) у відношенні перетинів реакцій i перетинів народження iзотопів i нейтронів у широкому інтервалі енергій від 11 MeV до кількох гігагеелектронвольт. Особлива увага приділялася даним щодо перетинів реакцій \( (n, xn) \). Встановлено, що вони грають визначну роль при виборі сполучень палива. Програма забезпечує дані щодо нейтронних перетинів, які узгоджуються з існуючими експериментальними даними, при цьому підкреслюється необхідність подальшої перевірки з використанням точних даних від прискорювача.