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Role of (n, xn) reactions in ADS, IAEA-benchmark and the Dubna Cascade Code*

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Abstract. Dubna Cascade Code (version-2004) has been used for the Monte Carlo simulation of the 1500 MW_t accelerator driven sub-critical system (ADS) with $^{233}U + ^{232}Th$ fuel using the IAEA benchmark. Neutron spectrum, cross-section of (n, xn) reactions, isotopic yield, heat spectra etc. are simulated. Many of these results that help in understanding the IAEA benchmark are presented. It is revealed that the code predicts the proton beam current required for the 1500 MW_t ADS for $K_{\rm eff} = 0.98$ to be 11.6 mA. Radial distribution of heat is fairly in agreement with other codes like the EA-MC and it needs nearly 1% less enrichment than given by other codes. This may be because the code takes care of the role of larger order of the (n, xn) reactions. It is emphasized that there is a strong need to study (n, xn) reactions both theoretically and experimentally for better design.

Keywords. Accelerator driven sub-critical system; IAEA Benchmark; Cascade Code; spallation neutron; simulation, (n, xn) reaction cross-section; heat; isotopic yield.

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1. Introduction

According to the IAEA-neutronic benchmark [1], the accelerator driven sub-critical system of 1500 MW_t power is supposed to be driven by 1 GeV proton beam. Nuclear densities of the fuel and structure components at the beginning of life (BOL) have been suggested in the given benchmark [1] with the demand of estimation of $K_{\rm eff}$ (for different ^{233}U-enrichments of the fuel) and the beam current. Also, estimations of heat and isotopic yield in different positions of the ADS are required. The whole exercise is fairly complicated from the point of development of a single simulation code which can generate cascades and provide transport of radiations in a multi-component medium, to keep account of the reactions and build up of $K_{\rm eff}$ including

*This talk is dedicated to the fond memory of late Professor V S Barashenkov, JINR, Dubna the burn-up, estimation of the heat etc. This becomes even more serious when the available data of neutron cross-sections beyond a few tens of MeV is scarce. During the last two years the Dubna Cascade Code has been modified successfully for the estimations of neutron yield in the spallation target [2,3], heat [4] and the isotopic yield [5–7] in the thin targets although without the inclusion of 'burn-up'. The code gives average value of $K_{\rm eff}$ in saturation region after lapse of early stage of generation.

In contrast to a conventional reactor, in ADS (n, xn) reactions have important role to play. In a conventional reactor, fission cross-section is highly dominant at thermal energies as compared to the (n, xn) reactions but in the presence of a spallation source and the fertile fuel, fission cross-section of the fuel is comparable to that of the (n, xn) reaction and that affects both neutron regeneration and heat production along with other problems related to the spatial distribution of heat and shielding. Cross-section of (n, xn) reactions and neutron yield given by Dubna Cascade Code for the given system have been used to study the heat and the isotopic yield. Based on these estimates, suitable beam current, $K_{\rm eff}$, relative percentage of ^{233}U/^{232}Th and number of escape neutrons have been determined for a 1500 $\rm MW_t$ reactor.

2. Dubna Cascade Code

2.1 (n, xn) *Reactions*

Dubna Cascade Code provides mathematical modeling of physical processes taking place in a multi-component medium on transport of radiation and beams of particles and heavy ions. It includes intranuclear pre-equilibrium-evaporation-fission model of Barashenkov and Toneev [8] which has recently been modified for evaporation and fission [5–7] in its 2004 version. In context of simulations given in this work it is important to mention that material density of a particular zone is considered to be constant and 26 group cross-section library due to Abagian *et al* [9] for the low energy and BARPOL for high energy have been used. In the past, the code has been tested in a number of ways, i.e. comparison of models of neutron production, experimental data of neutron and isotopes etc. and a great deal of such studies can be seen in ref. [4] and references therein. Some results of cross-sections related to present discussion of IAEA benchmark are highlighted here. In figures 1a and 1b cross-sections of (n, xn) reactions evaluated from the production cross-section divided by the neutron multiplicity for the ^{232}Th and ^{233}U targets estimated by the code have been displayed.

The figure does not carry data below ∼10.5 MeV because of the fact that 26 group library [9] does not include data of (n, xn) reactions below 10.5 MeV. It did not make much difference in the earlier years as at this energy only few data points of selected nuclei and that of only $(n, 2n)$ and $(n, 3n)$ reactions were known. In the near future we intend to update the library. Besides the data displayed in figure 1, we have obtained data of (n, xn) reactions for different materials of constructions, C, O, Fe, Cr, As, Pb, Bi etc. and compared with the experimental data [7,10] but could not present them due to limited space. It may however be mentioned that

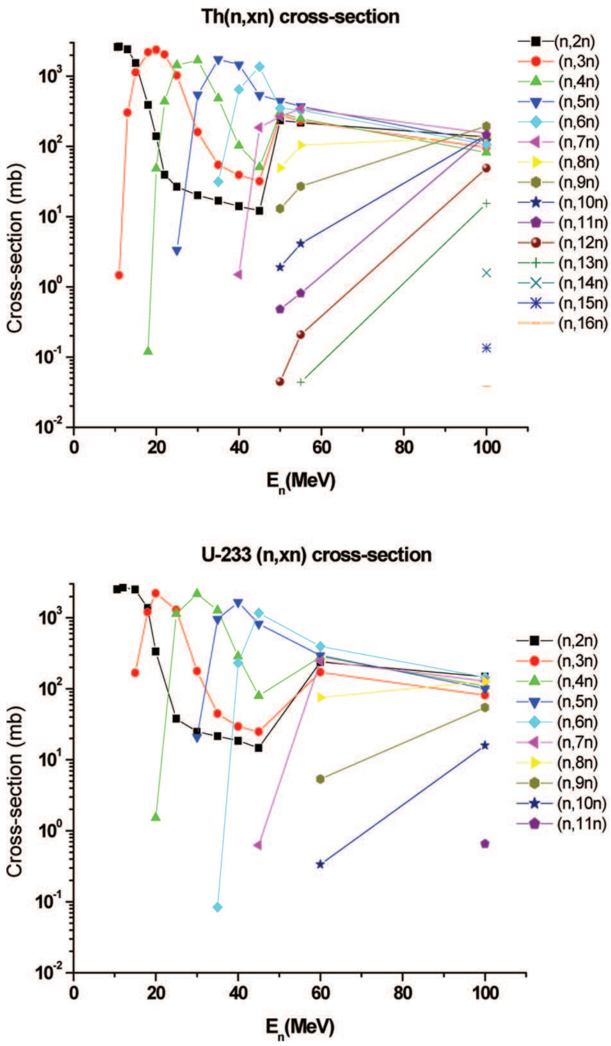

Figure 1. Cross-sections of (n, xn) reactions for ^{232}Th and ^{233}U from the Cascade-2004 Code.

the cross-sections given by the code are fairly in agreement at neutron energy from 10.5 MeV up to several hundreds of MeV (see Manish *et al* of this proceedings).

3. Isotopic yield

In the Cacasde-2004 version more exact formulae of level density have been used [11]. Also, fragments heavier than alpha masses are included as used in the generalized evaporation model. Similarly, fission model due to Fong [12] has been modified

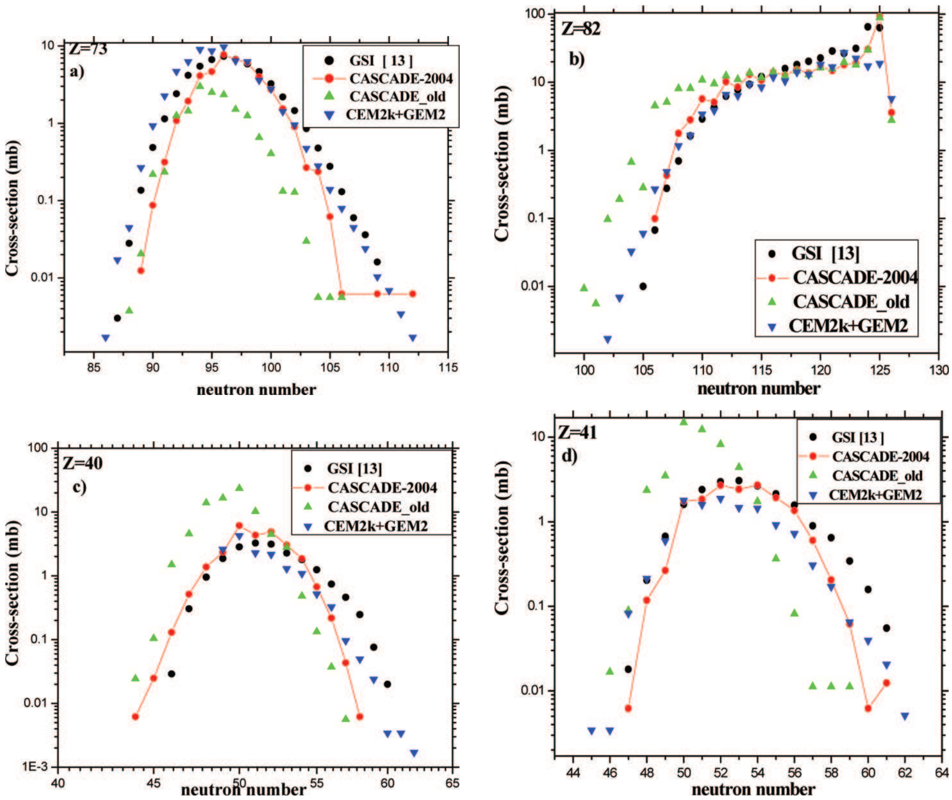

Figure 2. Comparison of experimental spallation products (for $Z = 73$ in (**a**) and $Z = 82$ in (**b**) and fission products (for $Z = 40$ in (**c**) and $Z = 41$ in (**d**)) with Dubna Code-old, 2004 versions and CEM2k+GEM2 code. Experimental data for both are from GSI [13].

using temperature or excitation energy dependence of the level density at the saddle point.

In figures 2a–2d experimental data of spallation yield of nuclei with $Z = 73$, 82 and fission yield with $Z = 40$ and 41 produced in 1 GeV p+Pb interaction [13] have been compared with the old and new versions of the Dubna Code along with the CEM2k+GEM2 code by Mashnik and Sierk [14]. It is evident that the Code version-2004 is much improved than its old version and our general impression is that it is quite comparable with that of the CEM2k+GEM2 code.

4. IAEA-Benchmark and simulation

In figure 3 cross-sectional view of the ADS benchmark design [1] has been shown and its compositional details, i.e. nuclei densities (BOL at 20°C) of five regions have been given in table 1 which shows that in regions 1 and 2 total fraction ^{233}U and ^{232}Th have been given without their break-up to individual proportion and by

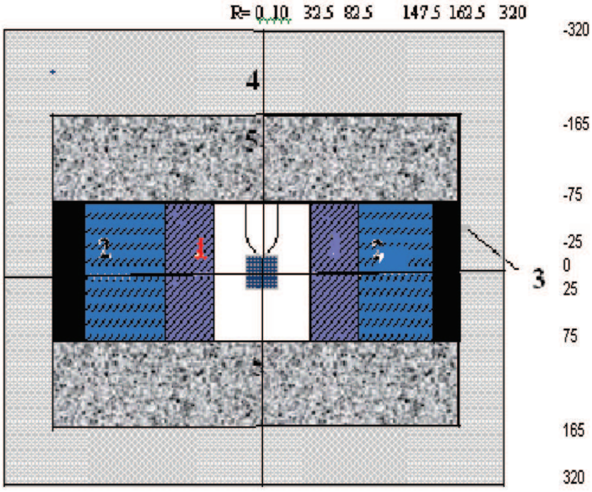

Figure 3. Cross-sectional view of the ADS benchmark design. The whole structure is in cylindrical shape of $2R \times L = 640 \times 640$ cm^2.

Table 1. Nuclei densities (BOL at 20°C) of elements in the five regions.

Nuclei	Region 1	Region 2	Region 3	Region 4	Region 5
^{232}Th	–	–	7.45E-3	–	–
^{233}U+^{232}Th	6.35E-3	7.45E-3	–	–	–
O	1.27E-2	1.49E-2	1.49E-2	–	–
Fe	8.10E-3	8.87E-3	8.87E-3		6.63E-3
Cr	1.12E-3	1.06E-3	1.06E-3		8.00E-4
Mn	4.60E-5	5.10E-5	5.10E-5		3.80E-5
W	4.60E-5	5.10E-5	5.10E-5		3.80E-5
Pb	1.77E-2	1.56E-2	1.56E-2	3.05E-2	2.41E-2

simulation one has to determine individual proportion for the required values of K_{eff}. In region 3 only ^{232}Th is filled up which develops fission activity rather slowly with the passage of time. Region 4 has thick lead shield only while region 5 has plenum extensions of steel canings of fuel pins. The benchmark proposes spallation target to be a cylinder of lead (Pb-) of size $R \times L = 20 \times 50$ cm^2. The proton beam collides at -25 cm as shown in figure 3.

The space between the spallation target and region 1 is empty. Even if it is filled with target-coolant like Pb+Bi eutectic, it will make only a small difference from the point of neutronics.

It may be pointed out that simulation by the Dubna Code-2004 does not include the so-called 'burnup' process. However, for the simulation in the region of spallation target there is no requirement of 'burnup' except in the case of some of the produced isotopes. The simulation results without the 'burnup' also carry significance as one can use these results for the purpose of input to the burnup codes.

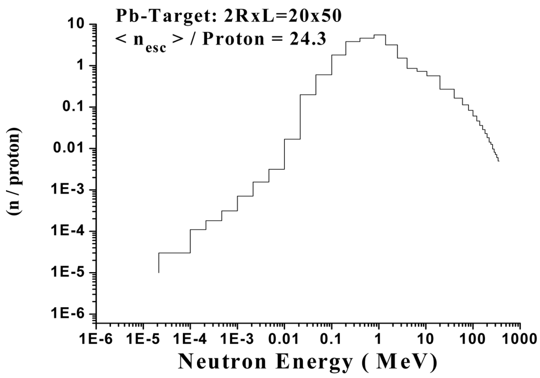

Figure 4. Energy spectrum of produced neutrons in 1 GeV p + Pb collision from the Dubna Code.

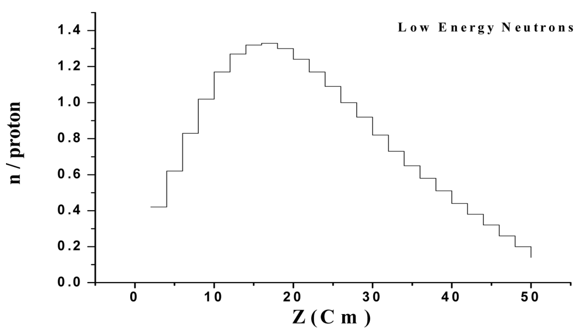

Figure 5. Spallation neutron distribution along the beam direction.

4.1 *Neutronics and heat distribution at BOL*

According to the Dubna Code-2004 version, 1 GeV proton beam produces 24.3 neutrons/proton and the energy spectrum of neutrons escaping from the spallation target is given in figure 4. The spectrum is peaked at 1 MeV and spreads from 2×10^{-5} to several hundreds of MeV. Neutron emission along the beam direction is not uniform and maximum neutrons are produced at the downstream distance of 15–16 cm as shown in figure 5 for neutrons with $E < 20$ MeV.

In table 2, results of simulation from the Dubna Code for the three compositional ratios ^{233}U/^{232}Th in regions 1 and 2 leading to characteristic values of $K_{\text{eff}} = 0.946$, 0.964 and 0.983 have been given. Requirement of accelerator current for the 1500 MW_t reactor is estimated to be 28.1, 18.1 and 11.6 mA for $K_{\text{eff}} = 0.946$, 0.964 and 0.983 respectively. The number of neutrons escaping from the whole assembly are estimated to be 0.6, 0.7 and 1.6 for the set-up with $K_{\text{eff}} = 0.946$, 0.964 and 0.983 respectively. In figure 6 heat density distribution in the radial direction of the assembly is given for the three cases. The point beam strikes at the $r = 0$ position. For the plot in figure 6a bin size of radial distance is chosen to be 10 cm. In order to study the bin size effect it is taken to be 4.65 cm in figure 6b. The heat deposited at this position in the three cases of K_{eff} is found to be proportional to the beam

Table 2. Results of simulation from the code.

	$^{233}U/^{232}Th$		
Density ratio in region 1	0.0127/0.1426	0.0132/0.1421	0.0137/0.1416
Density ratio in region 2	0.0113/0.1266	0.0117/0.1262	0.0121/0.1257
K_{eff}	0.946	0.964	0.983
N/P	429	617	1085
Heat (MeV)/proton	54000	79360	142600
Current (mA) for 1500 MW_t	28.1	18.1	11.6
Heat of reactor (MW_t) for 10 mA current	540	793.6	1426

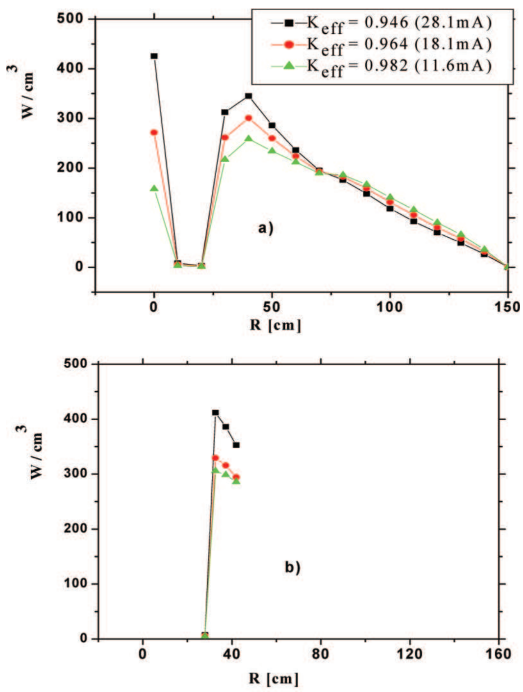

Figure 6. (**a**) Heat density distribution in radial direction of the whole assembly for bin size 10 cm. In (**b**) same plot is shown by reducing the bin size to 4.65 cm from 10 cm.

power density. The reactor heat density starts building up after radial distance 32.5 cm and attains the maximum within the first ∼5 cm. The maximum values are ∼412, 329 and 305 W/cm^3 for $K_{eff} = 0.946$, 0.964 and 0.983 respectively for the radial bin size of 4.65 cm (figure 6b). Finer details of bin size effect will be published elsewhere. At higher radial distances the distribution changes significantly at $r \sim 80$ cm because of the fact that the percentage of ^{233}U is higher in region 2 than in region 1 or it may be due to the anisotropy of heat distribution. Also, the percentage of slower neutrons increases in this region after passing region 1.

Table 3. Relation of ^{233}U/(^{233}U+^{232}Th)% and $K_{\rm eff}$ at the BOL obtained from the Dubna Code.

$K_{\rm eff}$	0.946	0.964	0.983
^{233}U/(^{233}U+^{232}Th)%	8.2	8.5	8.8

In table 3, percentage proportion of ^{233}U in the mixture ^{233}U + ^{232}Th (at BOL) has been given for $K_{\rm eff}$ obtained from the code. It may be pointed out that the percentage proportion of ^{233}U is significantly lower in Dubna Code for all the three $K_{\rm eff}$ values than the values obtained from the deterministic codes used at PSI (see details in ref. [15]) which used the JENDL 3.2 and JEF 2.2 libraries and the EA-MC code [15] itself. In general, both the PSI and EA-MC codes show disagreement (e.g. ratio being ∼9.5% in EA-MC and ∼9.9% in PSI code at $K_{\rm eff} = 0.98$) after using the same JENDL-3.2 library. Tucek *et al* [16] on using MCNP in KCODE mode have got even higher value (10.42%) at $K_{\rm eff} = 0.98$ compared to the PSI and EA-MC codes. This difference of enrichment in Dubna Code compared to other codes might be due to the following reasons: (i) the data libraries are different, (ii) early generations of neutron multiplication which show fairly higher value of $K_{\rm eff}$ than the saturation value at later generations (see figure 1 of ref. [16]), are not avoided in simulation by the Dubna Code, (iii) (n, xn) reaction cross-sections are well considered up to an extent in Dubna Code and neutron multiplication by these reactions may produce more number of fission reactions compared to that in other codes where (n, xn) reaction cross-sections might be smaller or neglected due to the unavailability of such data. The last possibility suggests that although there is smaller enrichment, there may be more fission reactions due to the larger number of secondary neutrons from (n, xn) reactions for the same power of ADS reactor. It may be expected that due to consideration of role of (n, xn) reactions the peak value of heat distribution at early distances may be lesser because a part of neutron energy is used in just producing (n, xn) reactions without fission but the spatial spread of heat distribution should be wider.

In figure 7 heat distribution in axial to radial direction of the ADS assembly of the said design has been shown for the three cases of beam energies, 400, 1000 and 2000 MeV. Different zones of heat densities are presented in different colors. Presently, this has not been compared with other code-results but there is a need for such comparison and discussions to understand the role of (n, xn) reactions in hybrid reactors.

5. Conclusions

The Dubna Code is useful to provide (i) neutron spectra, (ii) cross-sections of (n, xn) reactions (also see Manish *et al* of these proceedings), (iii) isotope and heat distributions for discussion of characteristics of ADS at BOL. The question of low enrichment of the fuel by the Dubna Code may be settled by detailed comparison of (n, xn) reactions with other codes. Inclusion of 'burnup' in the Dubna Code may have some bearing on this question. The work is in progress in this direction.

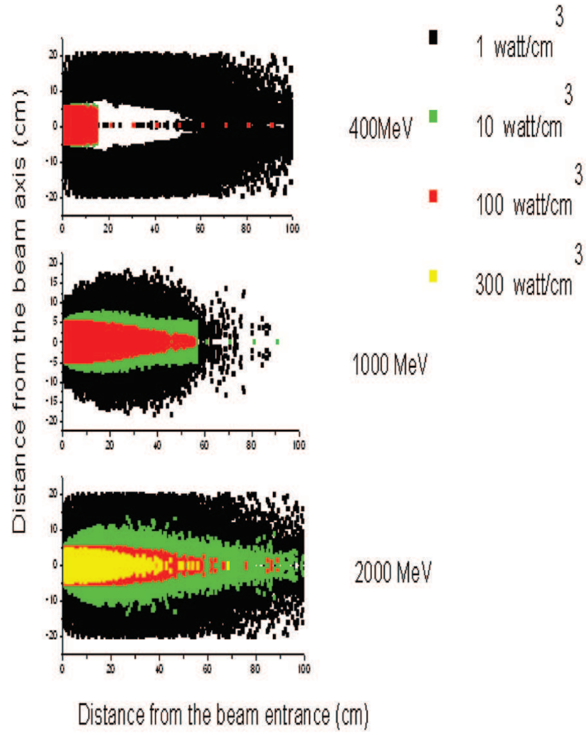

Figure 7. Heat zones of axial-radial direction at three proton-beam energies, 400, 1000, 2000 MeV obtained from the Cascade Code.

Acknowledgments

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Nomenclature

BARPOL: It is the cross-section library of high energy neutrons and abbreviated by names of Barashenkov and Polanski [17].
EA-MC: Energy amplification Monte Carlo code.

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