

Comparison of Different INC Physical Models of MCNPX to Compute Spallation Neutronics of LBE Target

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Abstract. Spallation particles can utilize in different fields such as neutron scattering studies, external source for burning spent fuel as well as running subcritical reactors. Different computational particle transport codes are widely used to model spallation process into the heavy targets. Among these codes, MCNPX 2.6.0 comprises various intra nuclear cascade models for spallation calculations. Impact of different intra nuclear cascade models on calculation of neutronic parameters of LBE target has been evaluated in this work. Escaped neutron yield, energy deposition and residual nuclei production in the spallation target has been calculated using the physical models. A comparison between the computational and experimental has been carried out to validate the computational data. The simulation data showed there is a good conformity between the obtained data from Bertini/Drenser and Isabel/Drenser. The data achieved by Bertini/Abla and Isabel/Abla models are close to each other for the studied parameters as well. Among the studied models, CEM showed more discrepancies with experimental and other computational data. According to the obtained data, INCL4/Drenser, INCL4/Abla and Isabel/Drenser models can meet more agreements with experimental data.

1. Introduction

The spallation target is ideally conceived to be high atomic mass material such as W, Ta, Hg, Pb, LBE (Lead Bismuth Eutectic) and U which are useful to yield high spallation neutron efficiencies and it is well known high density liquid metals like lead and LBE fit the requirement extremely well [1-3]. MCNPX 2.6.0 (Monte Carlo N-Particle transport code) is a general purpose Monte Carlo radiation transport code which involves different Intra-Nuclear Cascade models of Bertini, Isabel, INCL4 (Liège Intra-Nuclear Cascade) and CEM (Cascade-exciton model) for intra nuclear cascade (INC) calculations along with Drenser (associated with RAL (Rutherford Appleton Laboratory) or ORNL (Oak Ridge National Laboratory) fission models) and Abla for de-excitation [4]. Intra-nuclear cascade (INC) models are widely used to describe reactions between nucleon, pion or light ion projectiles with target nuclei. After the cascade an excited remnant nucleus is de-excited using evaporation/fission process. Some extended INC models have been reported in Table 1



Table 1.
Intranuclear cascade (INC) models' characteristic [5-8]

Physics process	Bertini	Isabel	CEM	INCL4
INC model	Bertini INC	Isabel INC	Improved Dubna INC	Cugnon INC
Nuclear density level	3	16	7	A nucleons - Positions shot in a Saxon-Woods density
Lower energy limit	20-150 MeV	20-150 MeV	~100 MeV	200 MeV
Upper energy limit	3.5 GeV for Nucl-Nucl 2.5 GeV for Pion-Nucl	1 GeV	5 GeV	2 GeV
The stopping criterium	Energy cut off	Energy cut off	Optical absorptive potential	Time cut off

In an accelerator driven system (ADS), high energy particles – usually protons above a few hundreds of MeV – are used to induce spallation reactions in the target. These kinds of reactions have been thoroughly investigated experimentally and theoretically using energetic proton beams by the researchers. Hence, ability study of different INC models introduced in MCNPX 2.6.0 for spallation neutronic calculations has been proposed in this work.

2. Material and methods

The spallation process has been modeled using MCNPX 2.6.0 code. A proton beam of 0.4, 0.6, 0.8 and 1 GeV energy has been used respectively to induce spallation reactions in LBE cylindrical target of 15 cm diameter and 60 cm thickness. A proton beam with a Gaussian intensity distribution of 0.2 cm FWHM has been used and the spallation neutron yield has been calculated using different physical models of Bertini/Drenser, Isabel/Drenser, Bertini/Abla, Isabel/Abla, INCL4/Drenser, INCL4/Abla and CEM. The models' effects on the energy deposition in the spallation target due to 1 GeV proton beam have been studied. F6 tally is used to calculate heat deposition into the spallation target. Residual nuclei production calculations have been carried out using the different physical models for the target bombarded by 1 GeV proton beam. Histp card has been used to calculate impurity production in spallation target. Residual masses have been transferred to pico gram (pg) per mA current scale by multiplying the NHTAPE data with A (mass number) $\times 1.036402\text{E-}08$ (g). To validate the calculations, the neutron yield achieved by the computational code using Bertini/Drenser, Isabel/Drenser, Bertini/Abla, Isabel/Abla, CEM, INCL4/Drenser and INCL4/Abla has been compared to experimental AECL (Atomic Energy of Canada Limited) where a Pb target was irradiated using a 960 MeV proton beam. In addition, the theoretical neutron yields were compared to the experimental data of BNL (Brookhaven National Laboratory) where 0.8, 1.0, 1.2 and 1.4 GeV protons were used. Manipulation of different INC models for residual nuclei calculations has been studied by reviewing of other carried out investigations extracted from the literatures to evaluate the most efficient INC model.

3. Result and discussion

3.1. Calculation of escaped neutron yield from the spallation target.

Figure 1 shows neutron yield calculation of the LBE target using different physical models indicated the obtained data using all the investigated physical models fit well each other at 0.4 GeV. Some relative discrepancies are observed at higher energies so that the higher the energy of the proton concludes in the higher the discrepancies between the results of the different models. At an energy of 0.6 GeV, the minimum value belongs to INCL4/Drenser and the maximum value belongs to both

Isabel/Abla and CEM with about 12% relative discrepancy between the maximum and minimum values. Calculations based on the CEM model result in the largest neutron yields for the entire energy span. Isabel/Abla, Bertini/Abla and CEM data have relatively closer agreements than the others at the total investigated energy span whereas the obtained neutron yields were the largest than the others as well. Bertini/Drenser and Isabel/Drenser data resulted in good agreements as well. The lowest values of neutron yield belong to INCL4/Drenser. In case of LBE target some disagreements has been observed between INCL4/Drenser and INCL4/Abla with maximum discrepancy of 5.8% at 1 GeV. (Fig. 1).

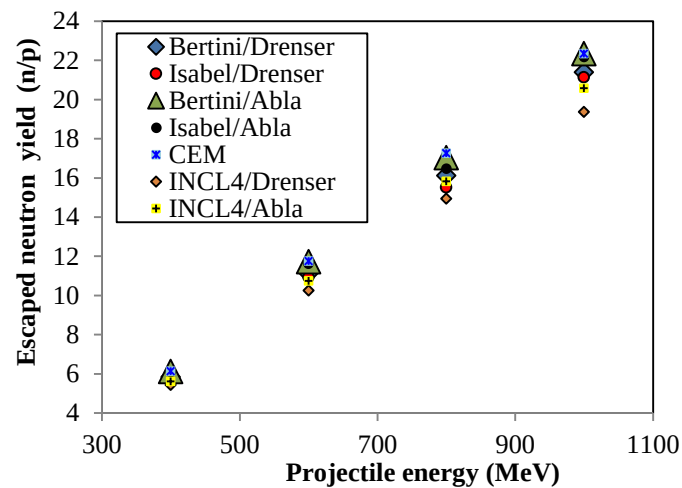


Figure 1. Comparison of different INC physical models in escaped neutron yield calculations of LBE target, the target diameter: 15 cm, height: 60 cm.

3.2. Calculation of deposited energy in the spallation target.

The energy deposition data achieved by 1 GeV proton irradiation of LBE target showed all the used models are in good conformity with each other in all length of the target (Fig.2).

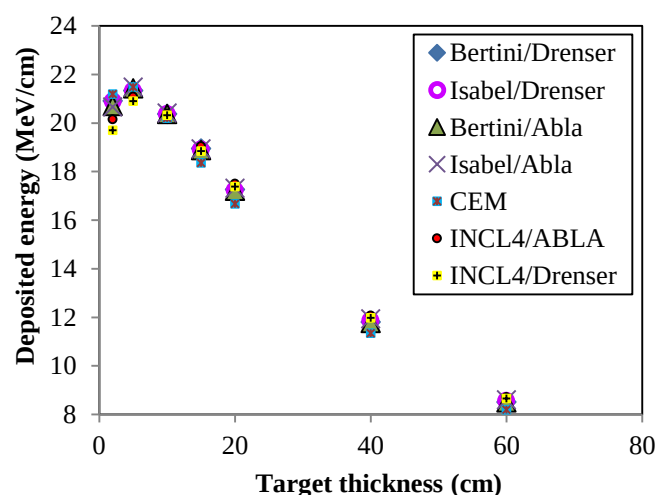


Figure 2. Comparison of different INC physical models for calculations of deposited energy in LBE target, the target diameter: 15 cm, height: 60 cm.

3.3. Calculation of residual nuclei production in the spallation target.

Calculations of residual nuclei production in a LBE target showed that the data obtained by Bertini/Drenser and Isabel/Drenser are in very good agreement as well as Isabel/Abla and Bertini/Abla result in very well-matched data with each other. The number of residual nuclei calculated using CEM model fits results of Isabel/Abla and Bertini/Abla data very well. These two groups' models (Bertini-Isabel/Drenser, Bertini-Isabel/Abla) have large discrepancies in evaporation as well as fragmentation region and small discrepancies in hot fission region. INCL4/Drenser show noticeably relative discrepancies in both hot fission and evaporation regions compared to the other data; in hot fission the model conclude in underestimated data than all of the other used models and in evaporation region the INCL4/Drenser data are overestimated than the others except Bertini/Drenser and Isabel/Drenser group. In case of INCL4/Abla this behavior is inversed so that in hot fission region the data are overestimated than all the investigated physical models and in evaporation region the obtained data are highly underestimated than all the studied physical models. In fragmentation region, INCL4/Drenser and INCL4/Abla data are close to each other and have fairly good agreements with CEM and Bertini/Abla-Isabel/Abla group. All the obtained data of different physical models have fairly good overlap in spallation region especially above A=175 (Fig.3).

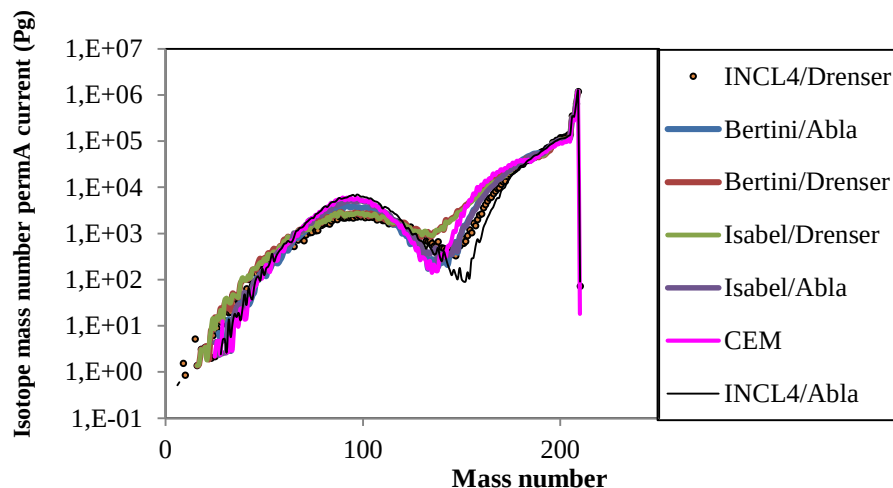


Figure 3. Comparison of different INC physical models for calculations of residual nuclei production in LBE target, diameter: 15 cm, height: 60 cm.

3.4. Comparison of experimental and computational neutron yield.

To evaluate confidence degree of computational and experimental data, a comparison between experimental neutron yield reported by AECL, BNL and theoretical data obtained by MCNPX 2.6.0 code calculations has been carried out for a Pb target [9-10]. Whereas experimental data on LEB was not available and Pb shows close neutronic behavior to LEB target [1], a comparison between the experimental data and the theoretical neutron yields obtained by the physical models used for a modeled Pb target with the same experimental dimension (10.2×61) has been done. The results showed that the INCL4/Drenser model can obtain more confidence data with experimental data for Pb target. Isabel/Drenser and INCL4/Abla models are also good in describing experimental values properly. The comparisons showed that there is a huge discrepancy between CEM INC model results and experimental data. The average relative discrepancies between experimental and theoretical data for Bertini/Drenser, Isabel/Drenser, Bertini/Abla, Isabel/Abla, CEM, INCL4/Drenser and INCL4/Abla models are 7.67, 5.68, 11.25, 9.13, 11.94, 3.74 and 5.60% respectively, $\text{discrepancy} = \left(\frac{\text{experimental} - \text{theoretical}}{\text{experimental}} \right)$. As the results show, the code data overestimated experimental data. According to the ACEL report, the experimental results obtained by the foil

activation method are believed to be accurate to within $\pm 5\%$. The computational obtained data in this work had an average uncertainty $< 0.7\%$.

3.5. Review of some carried out spallation simulations using different INC models.

Gorse-Pomonti et al. compared residual nuclei production in LBE target ($R=10$ cm, $L=100$ cm) irradiated by 1 GeV proton beam of 1 mA current [5]. Their data show there are good agreements between INCL4/Abla and Bertini/Drenser data except within the evaporation region where the Bertini/Drenser data is noticeably larger than the ones from INCL4/Abla. David et al. compared INCL4/Drenser, INCL4/Abla and Isabel/Abla models with experimental data for residual nuclei formation in Pb spallation target bombarded with 1 GeV and 0.8 GeV proton beams respectively. Their results showed that the data obtained using INCL4/Abla and Isabel/Abla models are in reasonable agreement with the experimental data while INCL4/Drenser model did not result in acceptable data especially in the hot fission region with about maximum 80% relative discrepancy. According to David et al. results, it can be seen the evaporation part of the charge distributions are not so well described by INCL4 and Isabel, but Isabel is better [11]. They reported this bad behavior could be due to a lack of excitation energy, since, on the one hand, the number of evaporated particles depends on the excitation energy, and, on the other hand, Isabel left the nucleus with higher excitation energy than INCL4. S. Leray has reported a comparison between Isabel/Drenser, INCL/Drenser and experimental data of residual nuclei formation via 1 GeV proton spallation reactions in Pb target [12]. Results of the investigations by Leray show the two INC models are fitting each other well except within the evaporation region and it is seen there is noticeable discrepancy between them and experimental data especially in the evaporation region and the hot fission region peak. In another report presented by Leray, the comparison between experimental and INCL4/Abla data achieved by irradiation of Pb target using 1 GeV protons shows the used model has acceptable agreements in the hot fission region while some noticeable disagreements has been observed in the spallation region [13].

4. Conclusion

In most of the carried out investigations of this work, CEM model presented some data with large relative discrepancy compared to the experimental data and the results of the other considered INC models. Isabel/Drenser and Bertini/Drenser data approximately overlap each other in neutron yield, energy deposition and residual nuclei calculations. Isabel/Abla and Bertini/Abla present roughly well-matched data in the case of the mentioned parameters. The lowest discrepancy with experimental neutron yield can be obtainable using INCL4/Drenser and Isabel/Drenser models. According to the other carried out studies these two models are more successive for residual nuclei and energy deposition calculations as well. However, more complementary benchmarks on wide range of the spallation targets with different material and dimension as well as wide range of projectile energy for spallation process induction in the target can validate the best INC model for such calculations.

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