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THEORETICAL SIMULATION OF RESIDUAL NUCLIDE PRODUCTS IN $^{208, 207, 206}$PB, ^{NAT}PB AND ^{209}BI (P,X) REACTIONS AT INTERMEDIATE AND HIGH ENERGIES

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THEORETICAL SIMULATION OF RESIDUAL NUCLIDE PRODUCTS IN $^{208, 207, 206}$PB, ^{NAT}PB AND ^{209}BI (P,X) REACTIONS AT INTERMEDIATE AND HIGH ENERGIES

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The independent and cumulative measured yields of residual products in thin lead and bismuth targets irradiated with 0.04-2.6 GeV protons are compared with results by the LAHET, CEM03, LAQGSM03, INCL+ABLA, CASCADE, and YIELDX codes, in order to evaluate the predictive power of the codes in this energy region. We found that the predictive power of the tested codes is different but is satisfactory for most of the nuclides in the spallation region, though none of the codes agree well with the data in the whole mass region of product nuclides and all should be improved further. On the whole, the predictive power of all codes for the data in the fission and fragmentation product regions and, especially, at the borders between spallation and fission and between fission and fragmentation regions is much worse than in the spallation region; therefore, development of better evaporation/fission/fragmentation models is of first priority.

INTRODUCTION

A number of current and planned nuclear projects, such as transmutation of nuclear wastes with Accelerator-Driven Systems (ADS) require a large amount of nuclear data. It is impossible to measure all the data, therefore reliable models and codes are needed to provide unmeasured cross sections in simulations for these projects. The codes to be used in such simulations should be verified, validated, and benchmarked against as much as possible reliable measurements.

During 2002 - 2004, under the ISTC Project # 2002 [1], ITEP has realized an experimental program to measure the residual nuclide production cross sections in $^{208, 207, 206}$Pb, ^{nat}Pb and ^{209}Bi thin targets irradiated with protons of 0.04, 0.07, 0.10, 0.15, 0.25, 0.4, 0.6, 0.8, 1.2, 1.6 and 2.6 GeV. Details of our measurements are described in [2- 4] and the obtained experimental results are briefly summarized in [5]. In the present work, we analyze all our measured data with six codes used in many applications in order to validate their predictive powers for our reactions.

THEORETICAL MODELING

Six codes were used to calculate our measured cross sections:

1. LAHET [6]is a well known and one of the most widely used in different nuclear applications code. It involves Monte-Carlo modeling of transport of nucleons, pions, muons, light ions, and antinucleons in extended objects or thin targets (interactions with nuclei). LAHET was developed at Los Alamos National Laboratory and includes several options of models to chose from to simulate the intranuclear cascade (INC), preequilibrium, evaporation, and fission of nuclei. The Bertini and ISABEL INC, Multistage Preequilibrium Model (MPM), Dresner's evaporation, and Atchison's (RAL) fission models (see details and references in [6]) are used in the present work.

2. CEM03 is the last, 2003, version of the improved Cascade-Exciton Model (CEM) [7] proposed initially at JINR, Dubna [8]. It has a longer cascade stage, less preequilibrium emission, and a longer evaporation stage with a higher initial excitation energy compared to its precursors CEM97 and CEM95. It is based on an improved [9] Dubna INC, extended Fermi break up and coalescence models from [10], and includes an improved version of the Generalized Evaporation-fission Model (GEM2) by Furihata [11]. CEM03 and/or its precursors are incorporated into the MARS, MCNPX, and LAHET transport codes and are used in many applications.

3. LAQGSM+GEM2 is a further development [12] of the Los Alamos version of the Quark-Gluon String Model [13] based of the Quark-Gluon String Model (QGSM) realized initially at JINR, Dubna [14]. It includes an improved version [9] of a time-dependent Dubna intranuclear cascade model, often referred in the literature simply as the Dubna intranuclear Cascade Model (DCM) [10] that makes use of experimental elementary cross sections (or those calculated with the Quark-Gluon String Model [14] for energies above 4.5 GeV/A), the improved pre-equilibrium model from CEM03 described above, refined versions of the Fermi break-up and coalescence models from [10], and an improved version of the Furihata's Generalized Evaporation-fission Model (GEM2) [11] as realized in CEM03. Here, we use the last, 2003, version of the code LAQGSM+GEM2, named LAQGSM03 [15], that was incorporated recently into the MARS and LAHET transport codes and is currently being incorporated into MCNPX.

4. INCL4+ABLA[16,17] code is based on a recent version of the Liege INC by Cugnon et al. [16] merged with the GSI evaporation/fission model ABLA by Schmidt et al. [17]. This code system was developed in the framework of the HINDAS project, it was incorporated into LAHET3 and MCNPX transport codes, and is widely used at present in Europe.

5. CASCADE is a transport code system developed at JINR, Dubna [18]. It allows to calculate nuclear reactions both on thin and thick targets and includes a time-dependent INC (different from [10]), the preequilibrium and evaporation models of CEM [8], and the Fong statistical fission model. It is under further development at JINR; its different modifications are used at present in many nuclear applications, mainly in the Former USSR.

6. YIELDX [19] is a simple and fast code based on semi-phenomenological systematics developed by Silberberg for product yields from proton-induced reactions. Its last version considers also neutron-induced reactions; it is widely used in many application, especially, by the astrophysical community.

The modeling was carried out at 25 energies from 0.03 to 3.5 GeV to produce smooth excitation functions (EF). At least half of a million protons were simulated each time to reach a proper statistics. To make the comparison to experimental data (ED) correct, the required cumulative yields were calculated on the base of simulated independent yields. The metastable products were not simulated. We compared simulated and experimental EF both qualitatively (plots) and quantitatively. For our qualitative comparison, 860 figures (172 products * 5 targets) with EF by the six codes and ED obtained by us under the ISTC Project #2002 as well as the measurements from [20] (for comparison) have been drawn. All our figures are presented in [21] and part of them, in [5], therefore we show here only Figs. 1 and 2 with several examples. For our quantitative comparison, we chose the mean simulated-to-experiment squared deviation factor <F> with its standard deviation <R>, as described in [2,3]. One example of our results for <F> averaged over all incident proton energies for the target ^{nat}Pb is shown in Fig. 3. We consider such a comparison quite effective, as it provides a quantitative picture of a general (averaged) agreement between calculations and all our data at all energies (the near the value of <F> to one, the better "the general" agreement of a particular code with the data).

To understand how different codes agree with the data in different nuclide production regions, we divided conventionally all products into four groups: shallow spallation products ($A>170$), deep spallation products ($140<A<170$), fission products ($30<A<140$), and fragmentation products ($A<30$). Note that such a division is conditional to some extent, as, for instance, at proton energies above 1 GeV, deep spallation products extend to mass A~120 and bellow, overlapping with fission products (^{127}Xe, for example, is produced by both spallation and fission at energies above 1 GeV). As an example, Tab. 1 presents averaged mean deviation factors <F> for the target ^{nat}Pb for all these four conventional regions separately. From Fig. 3, Tab. 1, and very many other results not shown here due to limited size of this paper we can conclude:

1) $A>170$: Most of the products from this region are predicted satisfactorily, with a mean deviation factor less than 2. Deviations above a factor of two are observed, as a rule, for independent yields (e.g., for ^{192}Ir), for (p,xn) reactions, and for near-threshold energies. Also, the deviations be-

tween ED and simulated EF's as well as between results by different codes increase at energies above 1 GeV. The near-target products (A above 200) are predicted variously at different proton energies: For instance, CEM03 predicts such products with <F> ~1.5 at energies bellow 1 GeV, but underestimates them significantly (<F>~6) at energies above 1 GeV. On the contrary, LAHET and LAQGSM predict these products with <F> ~ 1.5-2 at energies above 0.1 GeV, but fail to do so well at lower energies (<F> ~ 4 – 5). The same is true for INCL+ABLA: <F> ~ 1.3-1.5 at $E_p > 0.1$ GeV, <F>~6 at $E_p < 0.1$ GeV.

2) 140<A<170 (deep spallation products). With decreasing the mass of the products (excitation energy after the intranuclear cascade stage of a reaction increases), the predictive power of all the codes also decreases. The degradation of the predictive power of different codes varies. For example, for LAHET, <F> increases up to only 2.2; for LAQGSM, <F> increases up to 2.5; for YIELDX, <F> increases up to ~3; and in the case of INCL+ABLA , <F> increases up to 6. The INCL+ABLA underestimates significantly the deep spallation products overestimating their threshold energies. Note also that the thresholds of some reactions predicted by different codes may vary by up to hundreds of MeV. For example, the threshold for the production of ^{146}Eu predicted by different codes varies from 600 to 1200 MeV. On the whole, it seems to us that LAHET predicts most adequately most of the measured reaction thresholds in comparison with other codes tested here.

3) Fission products (FP) present about a third of all measured and analyzed here nuclides, and are described by the codes worse than the spallation products. The deviation between ED and simulated EF's as well as between different calculations themselves are much bigger than for the spallation products. LAHET and CEM03 show the best stability of the predictive power for fission products with <F> from 1.5 to 3. LAQGSM shows somewhat bigger deviation from ED (<F> up to 4), however, the agreement is better in the 80<A<110 region, with <F> around 2. A peculiar agreement is demonstrated by the code INCL+ABLA: <F> is too high (up to 6) in the 120<A<140 region where FP's overlap with deep spallation products, however, its agreement becomes the best (<F> from 1.5 to 2.0) in comparison with other codes for fission products with A<120. YIELDX and CASCADE show the worst agreement on FP's (<F> up to ~ 20). Note that most of simulated EF's are below ED in the fission region, i.e. the fission mode seems to be underestimated by the codes. The agreement of calculations with the fission data varies with the proton energy. For example, INCL+ABLA underestimates FP's at energies from ~0.1 to ~1 GeV, shows a good agreement at ~1 GeV, and overestimates them at higher energies. CEM03 predicts most of FP at relatively low energies (< ~0.5 GeV) much better than at higher energies. Note that despite the fact that CEM03 and LAQGSM use the same models for evaporation and fission (an improved version of GEM2 [11]), their predictive power <F> and mean ratio <R> are different, and this difference depends on the proton energy and mass numbers of the products. This is because CEM03 and LAQGSM03 use different INC, and here we see a good example of how using different intranuclear cascades by some codes affects their final results.

4) The fragmentation products are significantly underestimated by all codes tested here. Only a few fragmentation products were measured and can be compared here with calculation results. These measured fragment yields are underestimated by an order of magnitude and more. As a whole, YIELDX results for these fragments are most closed to ED. However, ^{7}Be, in particular, is best predicted by CEM03 and LAQGSM.

Table 1. Mean squared deviation factors <F> for different ranges of ^{nat}Pb products in three energy groups: <0.1 / 0.1-1.0 / >1.0 GeV.

Products	LAHET	LAQGSM	CEM03	INCL	CASCADE	YIELDX
A>170	5.5/1.5/1.7	2.4/2.0/2.1	1.9/1.5/2.4	5.3/2.0/1.3	1.7/1.5/1.8	8.3/1.9/1.9
140<A<170	- /1.7/1.9	- /7.1/1.6	- /2.6/1.7	- /8.6/3.2	- /2.4/1.8	- /1.5/2.3
30<A<140	6.0/3.2/2.3	2.0/3.1/2.6	1.4/1.9/2.6	1.7/1.9/1.5 (A<120) - /1.6/6.4 (A>120)	62/15/5.5	110/9.8/7.0
A<30	- / - /167	- /40/18	- /9.8/12	- / - /49	- / - /170	- /10.2/3.5

Finally, we like to mention that as the gamma-spectrometry method used to obtained all experimental data analyzed here allows to measure only part of the products from a nuclear reaction, our comparison can not pretend to be universal and to choose the best from the tested codes. Rather, it points on some separate problems each code still has, helping the authors of the codes to further improve them. The recent analysis [22] of the GSI measurements with essentially the same codes we used here confirms the conclusions of our present work.

CONCLUSIONS

The predictive power of the tested codes is different but was found to be satisfactory for most of the nuclides in the spallation region, though none of the benchmarked codes agrees well with all data in the whole mass region of product nuclides and all codes should be improved further. On the whole, the predictive power of all codes for the data in the fission product region is worse than in the spallation region; the agreement is even worse in the fragmentation region and on the border between spallation and fission regions. Therefore, development of better evaporation/fission/fragmentation models is of first priority.

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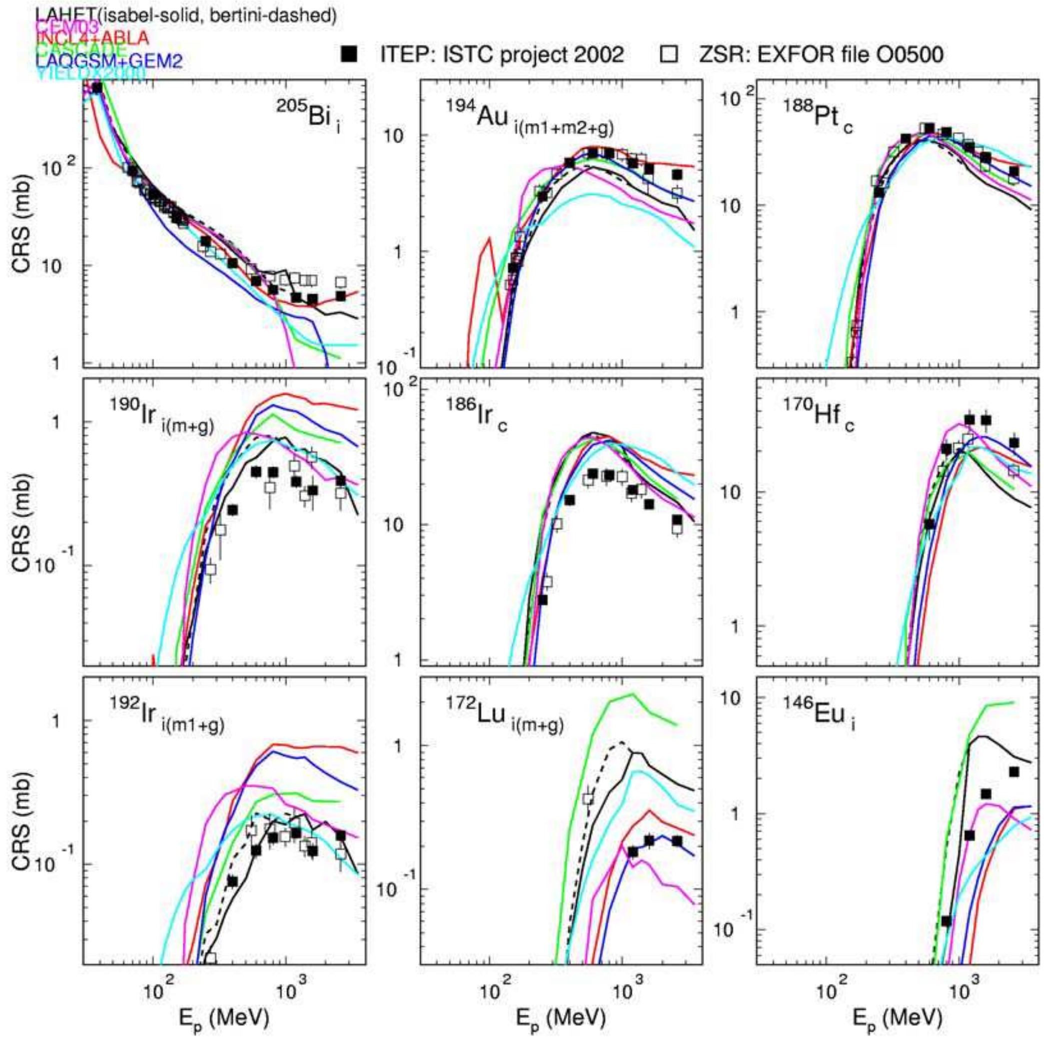

Fig. 1. Example of excitation functions for the ^{nat}Pb target calculated by the codes compared with our ITEP and ZSR [21] measurements.

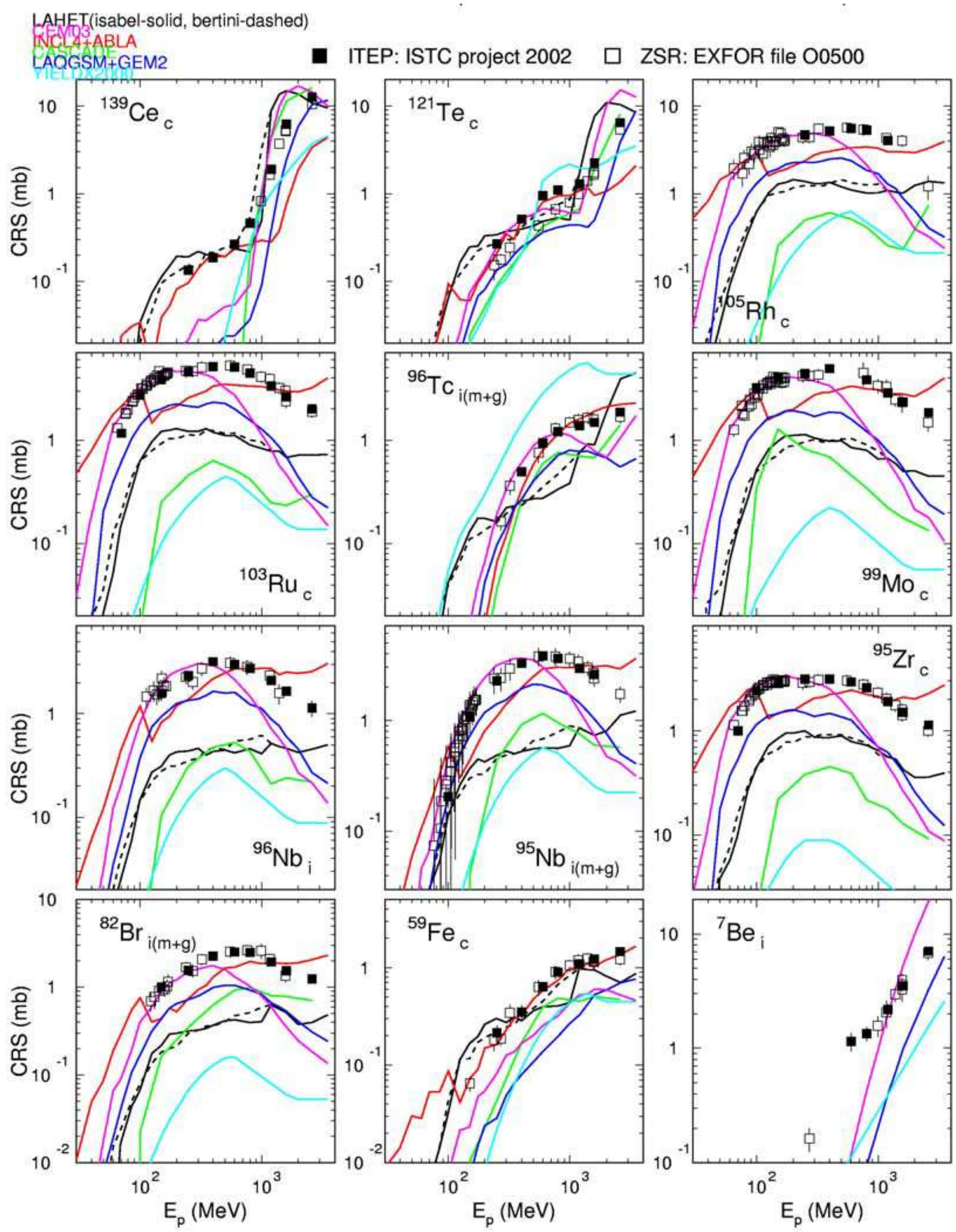

Fig. 2. Example of excitation functions for the ^{nat}Pb target calculated by the codes compared with our ITEP and ZSR [21] measurements.

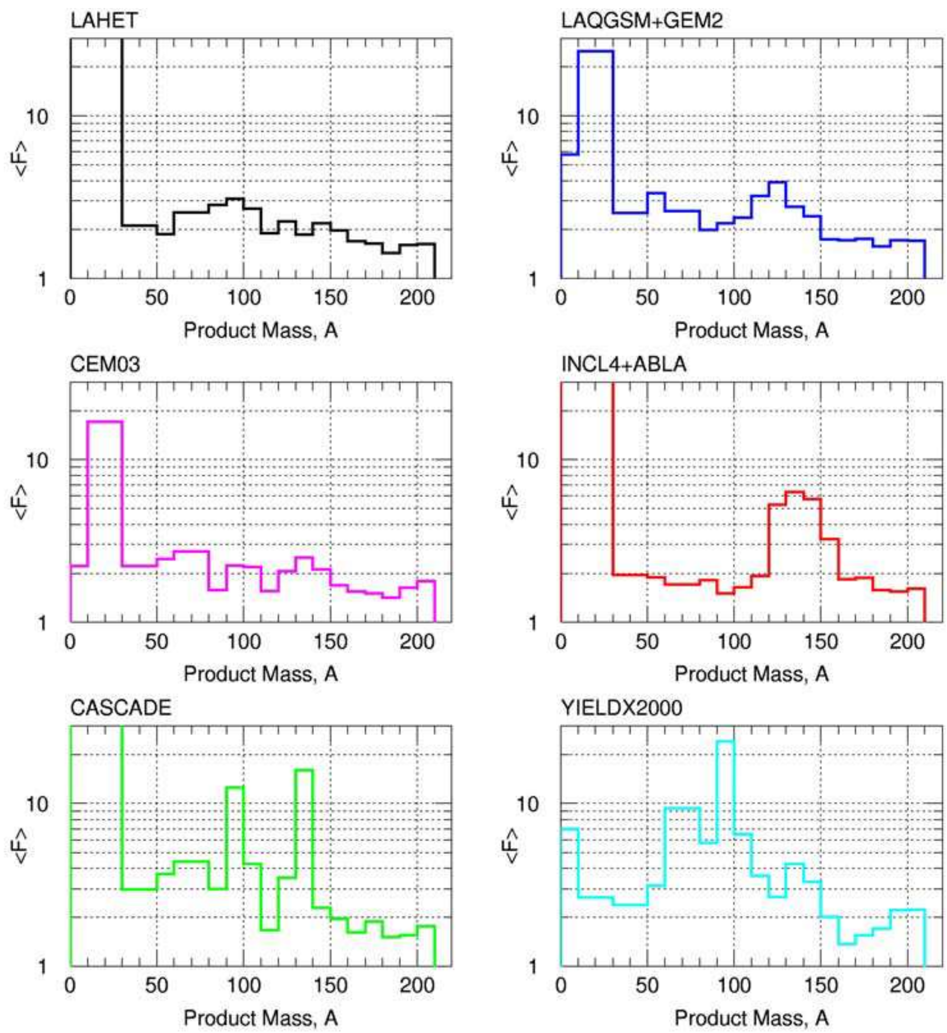

Fig. 3. Mean squared deviation factor <F> as a function of mass number of the products from ^{nat}Pb, averaged over all incident proton energies.