RECENT IMPROVEMENTS OF SPALLATION MODELS FOR BETTER PREDICTIONS OF HELIUM AND TRITIUM PRODUCTION

S. Leray[1)], A. Boudard[1)], J.C. David[1)], S. Lemaire[1)], Y. Yariv[1)], J. Cugnon[2)], T. Aoust[2, 3)], A. Kelic[4)], K.H. Schmidt[4)], M.V. Ricciardi[4)]

[1)] CEA/Saclay, DAPNIA/SPhN, 91191 Gif-sur-Yvette, Cedex, France
[2)]Liege University, Belgium, [3)] SCK-CEN, Mol, Belgium [4)] GSI, Darmstadt, Germany
Email: sylvie.leray@cea.fr

Reliable predictions of light charged particle production in spallation reactions are important to correctly assess gas production in spallation targets. The INCL4-ABLA combination of models, available in the MCNPX transport code, which was found to largely improve spallation residue predictions, was however not able to correctly predict light element yields. The work done recently on both the intranuclear cascade model INCL4 and the de-excitation model ABLA helps correct these deficiencies. In particular, it will be shown that the new versions of the codes coupled together now lead to much more reasonable predictions of both helium, which is important for assessing damage in the window, and of tritium production, which is a major contributor to the target radioactivity. Intermediate mass fragments which are observed experimentally can now be produced by the code.

I. INTRODUCTION

The objective of the NUDATRA domain in the EUROTRANS European FP6 project[1] is to provide improved simulation tools for ADS transmuters. In particular, it includes the improvement of nuclear models in the 200-1000 MeV energy range, their validation on experimental data and implementation into high-energy transport codes. The final goal is that most quantities related to high-energy reactions required for future ADS design, but also more generally for spallation sources, can be calculated as reliably as possible.

In the former FP5 HINDAS project[2], an important effort had been devoted to the collection of high quality experimental data and, simultaneously, to the development of improved spallation models. As a result of this work, the combination of the intranuclear cascade model, INCL4[3], and de-excitation model, ABLA[4], has been tested against all the available data and shown to give globally better predictions than models used by default (Bertini-Dresner[5]) in high-energy transport codes such as MCNPX[6]. INCL4-ABLA is now available in MCNPX and will soon be available in GEANT4. However, while the situation regarding predictions with INCL4-ABLA of neutron emission, heavy evaporation and fission residues production could be considered as satisfying, important deficiencies are still remaining when light evaporation residues and light charged particles are concerned[7]. It should be added that the model, as the other ones included into MCNPX, do not predict any intermediate mass fragments, whereas those are experimentally observed.

Reliable estimations of helium and tritium production are important for applications: helium is a concern in structural materials, in particular the window separating the accelerator vacuum and the spallation target, because it can lead to swelling and embrittlement; tritium can escape from the liquid target and cause problems for radioprotection. Therefore, some work has been devoted to the improvement of light composite particle prediction in both INCL4 and ABLA and will be presented in this paper.

II. PREDICTIONS OF THE MODELS PRESENTLY AVAILABLE IN MCNPX

Up to now, light composite particle production was only poorly predicted by the different models implemented into MCNPX. For helium out of iron, a systematic underprediction by a factor 2 to 3 by both INCL4-ABLA and Bertini-Dresner was reported in Ref. 7. For lead on the contrary, the models tend to overestimate the production (see fig. 5). Figs.1 and 2, which have been taken from Rapp et al.[8], show the cross-section for tritium production, respectively in lead and iron, as a function of the incident proton energy. Here, the results are compared with MXNPX calculations done using three different models: Bertini-Dresner (denoted Bertini-RAL in the figure), CEM from Ref. 9 and Isabel (from Ref. 10) plus Dresner (RAL). Since in ABLA only nucleons and alphas can be evaporated, INCL4-ABLA does not produce any tritium. It can be stated from the two figures that none of the tested models is able to account for the measured tritium production in both iron and lead. Only in the case of lead is Isabel-Dresner giving a reasonable agreement with the experimental data. Otherwise, discrepancies up to a factor five can be observed. Also, the dependence of the cross-section with the incident energy is sometimes not given properly. It should be noted that the experimental situation is also not totally satisfying since large discrepancies between different sets of data can be observed.

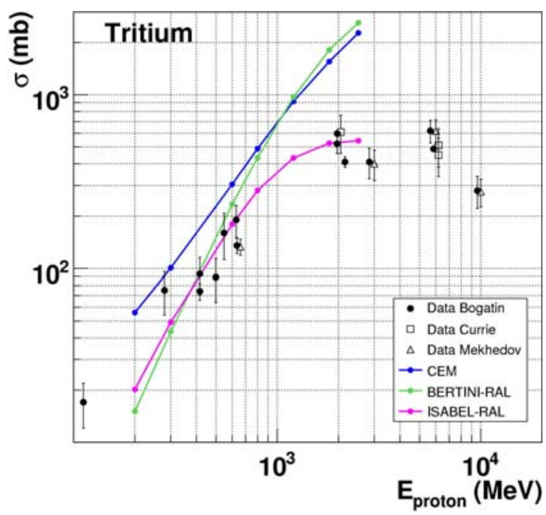

Fig. 1. Tritium production cross-sections in lead as a function of incident energy calculated with MCNPX using CEM, Bertini-Dresner (RAL) or Isabel-Dresner and compared with experimental data. From Rapp et al.[8].

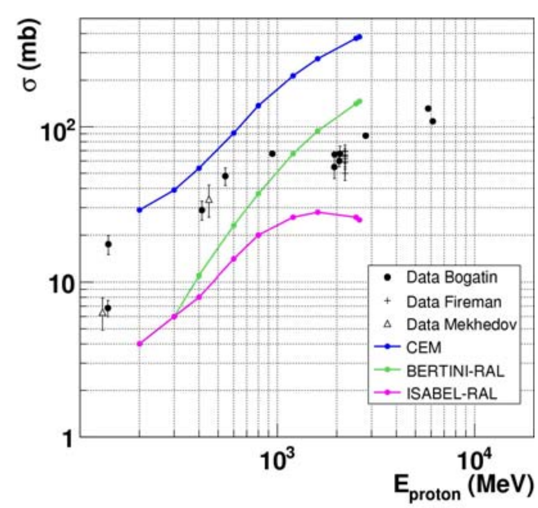

Fig. 2. Same as Fig.1 but for iron.

To illustrate the importance of predicting tritium production correctly, Fig. 3 (taken from Ref. 11) shows the results of a calculation of the MEGAPIE target done with MCNPX. The evolution of the total activity in the liquid lead-bismuth eutectic (LBE) after irradiation calculated with different models is plotted as a function of time. The results are very similar except around 10 years after irradiation where INCL4-ABLA disagrees with the other models. This is in fact due to the lack of tritium production in the evaporation model, as it can be checked by looking specifically at the activity due to tritium (dashed curve for Bertini-Dresner, line with crosses for INCL4-ABLA).

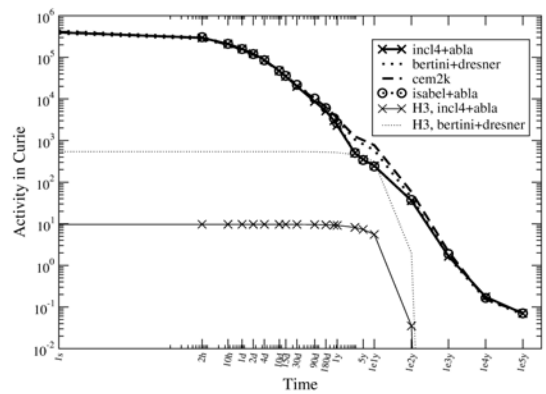

Fig. 3. Total activity (in Curies) of the LBE as a function of cooling time after 120 days of irradiation with 575 MeV protons at 1.4mA using different models in MCNPX. From Ref. 11.

III. IMPROVED LIGHT COMPOSITE PARTICLE PRODUCTION IN INCL4-ABLA

In light composite particle energy spectra two different components are generally observed: a low-energy isotropic one coming from the evaporation stage, and a high energy tail more forward peaked. An attempt to separate the two components has been done recently by Herbach et al.[12]. Fig. 4 is taken from Ref. 12 and shows the relative contribution of this high-energy component, called pre-equilibrium in this paper, relative to the total yields of the different light composite particles, versus the target charge, at 1.2 GeV. It can be seen that, while ^{4}He is produced predominantly by evaporation, for the other light composite particles the so-called pre-equilibrium contribution is far from being negligible, reaching even 60% for ^{3}He on high Z targets.

The level of this contribution in the production cross-sections of tritium and ^{3}He shows the importance of being able to account for the high-energy tail with the models.

This is the reason why light composite particle emission has been introduced in INCL4 in Ref. 13.

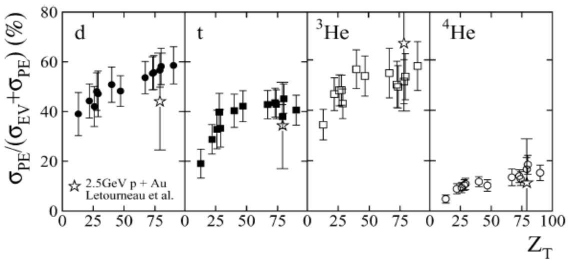

Fig. 4. Contributions of the pre-equilibrium emission relative to the total yield of light composite particles. The data measured for reactions with 1.2 GeV protons are plotted as a function of the atomic target number Z_T. From Ref. 12.

III.A. Cluster emission in INCL4

In Boudard et al.[13], a surface coalescence mechanism has been proposed to describe the emission of nucleon clusters during the intra-nuclear cascade stage and implemented into INCL4. It is based on the assumption that a cascade nucleon ready to escape at the nuclear surface can coalesce with other nucleons close in phase space and form a cluster. Two parameters have been introduced in the model: the volume of the phase space cell in which nucleons should be to form a cluster and the distance from the surface at which the clusters are built. When different clusters can be formed the priority is given to the largest one.

In Ref. 13 the model was found to give a reasonable agreement with the available data. However, the ratio between the different species of cluster was not totally satisfying. In the new version INCL4.4, the same priority has been given to t and ^{3}He, which was not the case previously, and the parameters have been chosen a little differently. Also, this version of INCL4 has been improved by introducing a potential for pions, allowing the nuclear potential to be isospin and energy dependent and by improving the correlation between coordinate and momentum spaces[14]. Calculations done with INCL4.4 coupled to the de-excitation model GEM[15] are compared with the experimental data from Ref. 11 in fig. 5. ABLA has not been used here since it does not produces d, t or ^{3}He clusters. It can be seen that the high energy tail is very well reproduced by the INCL4.4 model for all species of light charged particles at all angles. A similar agreement was obtained when comparing the model with p+Au data from Ref. 19 at 2.5 GeV.

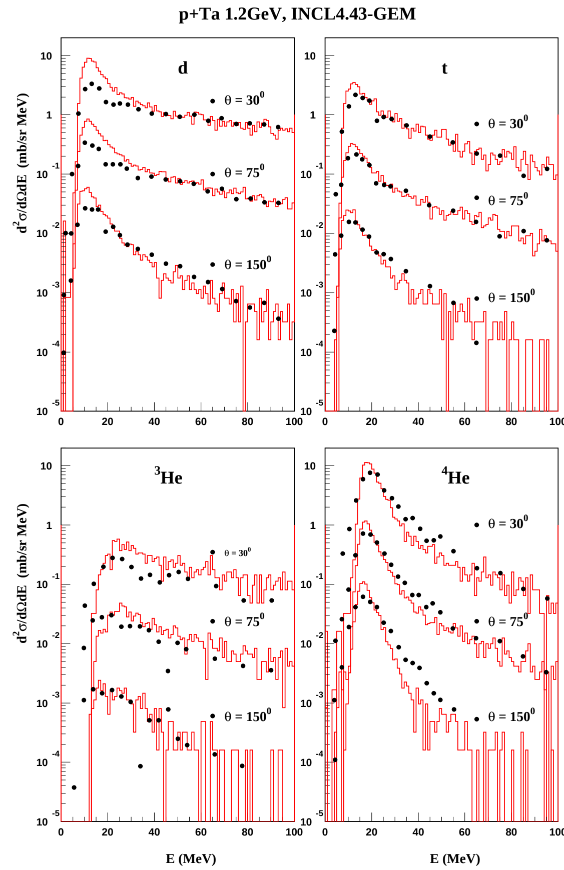

Fig. 5. Light composite particle double-differential cross-sections, in the p+Ta reaction at 1.2 GeV, measured by Ref. 12 and compared with the results of INCL4.4 coupled to the de-excitation model GEM.

III.B. Improvements of ABLA

Simultaneously to the work on INCL4, the authors of ABLA have produced a new improved version of the model, ABLA07[16]. This version now allows the evaporation of all the types of light charged particles from p to ^{4}He but also of Intermediate Mass Fragments (IMF). It uses improved parameterizations of inverse reaction cross-sections and barriers of potential in order to better reproduce experimental particle energy spectra. A simultaneous break-up (multifragmentation) mechanism has been added for systems with excitation energy exceeding 3 MeV per nucleon. The fission part has also been modified. Examples of the improved agreement with experimental data can be found in Ref. 16. In particular, it is shown that the de-excitation model is now able to correctly predicts IMF production cross-sections measured in the p+U reaction at 1 GeV. As regards the purpose of this paper, a rather good prediction of tritium and helium production is expected.

IV. CALCULATIONS WITH THE NEW VERSIONS

Since the new versions of INCL4 and ABLA are not yet coupled together, calculations of tritium and helium productions have been done by generating with INCL4.4 a file of pre-fragments with mass, charge, excitation energy and angular momentum that are used as inputs for ABLA07. Fig. 6 shows the result for the total helium production cross-section in iron as a function of proton incident energy compared to experimental data and to calculations with other models. Obviously, the new version represents progress compared to the previous one or to Bertini-Dresner. It should be noted that GEM coupled to INCL4.4 gives a similar agreement. The dashed curve gives the contribution of helium coming from the cascade stage. As discussed previously, it is rather small (10 to 20%) for helium since ^{4}He is dominating the total helium production.

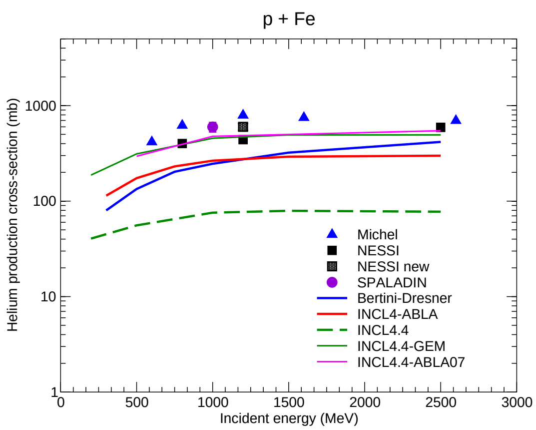

Fig. 6. Helium (^{3}He+^{4}He) production cross-sections in iron calculated with the new versions INCL4.4-ABLA07 (pink) compared to data measured by different groups (Refs. 17 to 20) and to calculations with INCL4-ABLA (red) and Bertini-Dresner (blue) models. The dashed curve is the contribution from the cascade cluster emission.

The new calculation also improves the prediction of ^{4}He production cross-sections from lead compared to the old version, as it can be seen in Fig.7. It seems to agree better with Leya et al.[18] than NESSI[12] data. It is the contrary for INCL4.4+GEM calculation.

Figs. 8 and 9 present the results obtained for the production of tritium on iron and lead targets respectively. In both cases, INCL4.4 coupled to either ABLA07 or GEM gives a reasonable agreement with the NESSI data at 1.2 GeV while it overpredicts the other sets of data.

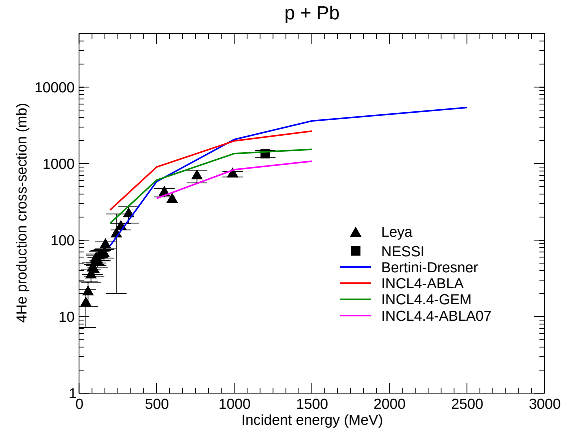

Fig. 7. Same as Fig. 5 but for ^{4}He production cross-sections in lead. Data from Refs. 12 and 18.

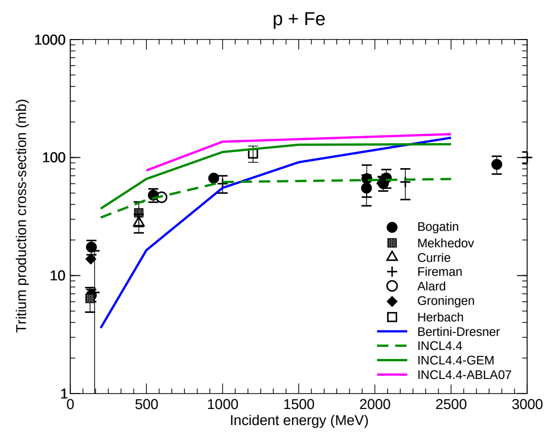

Fig. 8. Same as Fig. 5 but for tritium production cross-sections in iron. Data from Refs. 2, 12 and 21-25.

The contribution of tritium coming from the cascade stage is also shown. Here it accounts for a significant part of the total yield, more than 50% in the case of lead. However, it seems that our procedure to make clusters in INCL4 produces too many clusters at low energy. This was already observed in Ref. 14 when comparing double-differential particle energy spectra at low incident energy. The fact that the contribution of the high-energy tail is important may be an explanation of why some experimental data could be underestimated. Indeed, when measurements are done with telescopes, there is generally a high-energy threshold above which particles are not detected. In the case of NESSI data this high-energy tail has been well measured. Since the experimental situation is not clear it is nevertheless difficult to conclude.

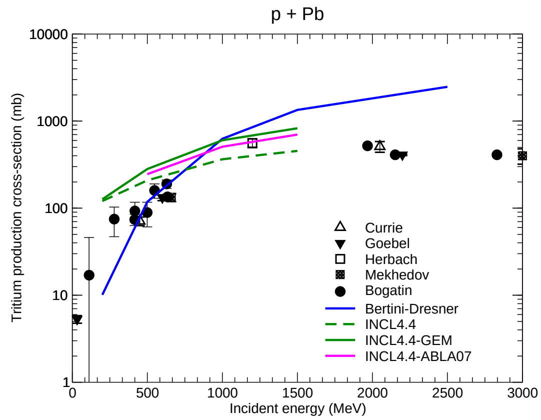

Fig. 9. Same as Fig. 5 but for tritium production cross-sections in lead. Data from Refs. 11, 21- 23, 26.

V. CONCLUSIONS

In this paper we have reported improvements brought to the models INCL4 and ABLA regarding the production of light composite particles. The inclusion of cluster formation through a coalescence procedure in phase space in INCL4.4 allows correct accounting for the high energy tail experimentally observed (except at low incident energies). INCL4.4 followed by the new ABLA07 version gives much better predictions of both helium and tritium production than models currently available in MCNPX. However, a quantitative estimation of the degree of agreement is difficult due to remaining discrepancies between different sets of experimental data.

INCL4.4 and ABLA07 will be soon coupled together and tested against a wide set of experimental data regarding spectra of neutrons, light charged particles, residues (including IMF), in order to check that the combination gives a better or, at least, a similar agreement than the old version. It will be then available for implementation into MCNPX or GEANT4.

ACKNOWLEDGMENTS

This work was partially supported by the European Community contract FI6W-CT-2004-516520.

REFERENCES

1. FP6 Euratom project EUROTRANS/NUDATRA, contract number FI6W-CT-2004-516520.
2. HINDAS final report, FP5 Euratom contract FIKW-CT-2000-00031, J.P. Meulders, A. Koning and S. Leray ed. (2005).
3. A. Boudard et al., “Intranuclear cascade model for a comprehensive description of spallation reaction data”, *Phys. Rev*. **C66** (2002) 44615.
4. A.R.Junghans et al., *Nucl. Phys.* **A629**, 635 (1998).
5. H.W. Bertini, *Phys. Rev.* **131**, 1801 (1963); L. Dresner, *ORNL Report ORNL-TM-196* (1962).
6. J.S. Hendricks et al., MCNPX 2.5.d, *report LA-UR-03-5916* (2003)
7. S. Leray et al., “Validation of high-energy nuclear models: state-of-the-art and perspectives”, *Nucl. Instr. Meth. Phys. Res.* **A562 (2)**, 806 (2006).
8. B. Rapp et al., “Benchmarking of the modelling tools within the EURISOL-DS project”, *Proceedings of International Workshop on Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF-8)*, Pohang, South Korea, May 22- 24, 2006.
9. S.G. Mashnik et al., *AIP Conf. Proceedings* **768**, 1188 (2005)
10. Y. Yariv and Z. Fraenkel, *Phys. Rev.* **C20**, 2227 (1979).
11. S. Lemaire et al., contribution to *Intern. Conf. on Nucl. Data for Science and Techn. (ND2007*), Nice, France, April 22-29, 2007.
12. C.M. Herbach et al., *Nucl. Phys.* **A765** (2006) 426.
13. A. Boudard et al., “A new model for production of fast light clusters in spallation reactions”, *Nuc. Phys.* **A740** (2004) 195.
14. A. Boudard et al., contribution to *Intern. Conf. on Nucl. Data for Science and Techn. (ND2007*), Nice, France, April 22-29, 2007.
15. S. Furihata, Nucl. Instrum. Methods Phys. Res. B 171 (2000) 251; S. Furihata, T. Nakamura, J. Nucl. Sci. Technol., Suppl. 2 (2002) 720, Tsukuba, Japan.
16. M.V. Ricciardi et al., contribution to *Intern. Conf. on Nucl. Data for Science and Techn. (ND2007*), Nice, France, April 22-29, 2007.
17. R. Michel et al., *Nucl. Instr. Meth. Phys. Res.* **B103**, 183 (1995); M. Gloris et al., *Nucl. Instr. Meth. Phys. Res.* **A463**, 593 (2001).
18. I. Leya et al., *Nucl. Instr. Meth. Phys. Res.* **B 229** (2005) 1.
19. M. Enke et al., *Nucl. Phys.* **A657**, 317-339 (1999).
20. E. Le Gentil et al., “Exclusive measurements on Fe-56+p at 1 A Gev with the SPALADIN setup at GSI”, *Nucl. Instr. Meth. Phys. Res.* **A562 (2)**, 743 (2006).
21. V.I. Bogatin, V.F. Litvin, O.V. Lozhkin, N.A. Perfilov, Yu.P. Yakovlev, *Nucl. Phys.* **A260**, 446 (1976)
22. B.N. Mekhedov, V.N. Mekhedov, *Yadernaya Fizika Vol.***11**, p.708 (1970)
23. L.A. Currie et al., *Phys. Rev*. **101** (1956) 1557.
24. E. L. Fireman and J. Zähringer, *Phys. Rev.* **107**, 1695 (1957)
25. J.P. Alard et al., *Il Nuovo Vimento, Vol.* **30a**, n°2 (1975)
26. K. Goebel, H. Schultes, J. Zähringer, Report CERN 64-12, 1964.