ELSEVIER

Journal of Nuclear Materials 307–311 (2002) 1710–1714

journal of nuclear materials

www.elsevier.com/locate/jnucmat

Advanced Monte Carlo procedure for the IFMIF d-Li neutron source term based on evaluated cross section data

S.P. Simakov [a,*], U. Fischer [a], U. von Möllendorff [a], I. Schmuck [a], A.Yu. Konobeev [b], Yu.A. Korovin [b], P. Pereslavtsev [b]

[a] *Forschungszentrum Karlsruhe, Institut für Reaktorsicherheit, Postfach 3640, D-76021 Karlsruhe, Germany*
[b] *Institute of Nuclear Power Engineering, 249020 Obninsk, Russian Federation*

Abstract

A newly developed computational procedure is presented for the generation of d-Li source neutrons in Monte Carlo transport calculations based on the use of evaluated double-differential d + ^{6,7}Li cross section data. A new code M^{c}DeLicious was developed as an extension to MCNP4C to enable neutronics design calculations for the d-Li based IFMIF neutron source making use of the evaluated deuteron data files. The M^{c}DeLicious code was checked against available experimental data and calculation results of M^{c}DeLi and MCNPX, both of which use built-in analytical models for the Li(d, xn) reaction. It is shown that M^{c}DeLicious along with newly evaluated d + ^{6,7}Li data is superior in predicting the characteristics of the d-Li neutron source. As this approach makes use of tabulated Li(d, xn) cross sections, the accuracy of the IFMIF d-Li neutron source term can be steadily improved with more advanced and validated data.

1. Introduction

The International Fusion Materials Irradiation Facility (IFMIF) [1] is an accelerator-based d-Li neutron source with the capability to produce neutrons at sufficient energy, intensity and irradiation volume to test samples of candidate materials up to a full lifetime of anticipated use in fusion energy reactors. The accuracy of the assessed induced radiation effects will be affected to a large extent by the quality of the predictions of spectral and angular neutron yield.

To enable neutronics calculations for IFMIF, the Monte Carlo code M^{c}DeLi has been previously developed [2]. It simulates the configuration of dual beams incident on the lithium target surface, the direction of each beam and the spatial intensity/current distribution to meet the requirements of the IFMIF project. The deuteron slowing down process in the lithium is described according to the well known empirical model of Ziegler et al. [3]. The neutron production via the Li(d, xn) reaction considers two competing reaction mechanisms: deuteron stripping and deuteron absorption followed by the formation of a compound nucleus with subsequent neutron emission. Free parameters of these models have been determined from fits to the angular–energy distributions of neutron yields from thick lithium targets, measured at 32 and 40 MeV incident deuteron energies. The subroutines simulating the deuteron beam configuration, the slowing down in the lithium and the Li(d, xn) reaction cross sections were linked to MCNP4B [4] to enable neutron transport calculations for the IFMIF test modules. More recently, the M^{c}DeLi code has been intensively tested against available experimental data for the full deuteron energy range from 5 to 50 MeV [5]. This test has shown that M^{c}DeLi fails to reproduce the data for deuteron energies below 30 MeV (break down at energies below 15 MeV) and the high energy part of the neutron spectrum above 40 MeV as well. In the deuteron energy range

* Corresponding author. Tel.: +49-7247 82 4997; fax: +49-7247 82 3718.
E-mail address: simakov@irs.fzk.de (S.P. Simakov).

0022-3115/02/$ - see front matter
PII: S0022-3115(02)01142-X

32–40 MeV, for which M^{c}DeLi was especially developed, the simplified Li(d, xn) reaction cross section modelling makes it difficult to further improve the quantitative agreement with the experimental data.

The Monte Carlo code MCNPX is a major extension to MCNP with the capability to simulate neutron and charged particle transport up to energies of a few GeV. The presently available version 2.1.5 [6] is not yet capable of using cross sections from evaluated data libraries for charged particles. Instead, it uses various nuclear models, which originally were developed for the intermediate and high energy physics domain. For relatively low incident energies (<150 MeV) and light target nuclei MCNPX assumes, as default, the ISABEL intranuclear cascade model. From the methodological point of view MCNPX 2.1.5 resembles the M^{c}DeLi code: both use built-in analytical models for the d-Li interaction. It is questionable, however, if the ISABEL model is able to predict the d-Li neutron source characteristics with sufficient accuracy as compared to M^{c}DeLi which was developed and fitted for this particular reaction and energy range. Nevertheless it is certainly reasonable to start testing MCNPX, since future extensions of the code are reported to be capable of using evaluated charged particle data libraries.

2. M^{c}DeLicious methodological approach

Drawbacks of the M^{c}DeLi approach can be overcome if the simplified semi-empirical model for the Li(d, xn) reaction is replaced by a complete and detailed description of the deuteron interactions with the lithium. This can be accomplished by the use of tabulated data from evaluated data files. Recently a newly evaluated d-Li data library [7] has been developed under a collaboration of INPE (Obninsk) and FZK (Karlsruhe). Diffraction theory and a modified cascade evaporation model have been applied for calculating the cross sections and the angle–energy distributions of the reaction products for deuteron energies up to 50 MeV. It turns out that over this energy range, a variety of reaction channels are open for the deuterons interacting with the lithium nuclei. In the INPE evaluation, all channels resulting in the emission of a specific kind of particles are summarized in cumulative particle yields, i.e. there are available in the file production cross sections such as (d, xn), (d, xγ), (d, xα), etc. For IFMIF neutronics calculations the emission of neutrons and γ-rays is of primary importance since the other particles are short ranged and will be stopped in the lithium target.

To take full advantage of the tabulated d + ^{6,7}Li data, a special routine was developed to read and process the cross sections from the files. As a preparatory step, the ENDF-6 formatted data were processed with the ACER module of the NJOY-99 code [8] into the ACE format suitable for a Monte Carlo sampling scheme. The sampling procedure is as follows. The deuteron track length is sampled, taking into account the total d-Li interaction cross sections read from the file; then for the given deuteron energy the interaction probability with either of the ^{6}Li and ^{7}Li nuclides is calculated according to their macroscopic cross sections. Eventually the energy and angle of the generated neutron and photon are sampled. This information together with the coordinates of the d-Li collision site inside the lithium target cell is further used for the transport calculations of the neutrons and photons. To enable full neutronics calculations for the IFMIF neutron source, this procedure has been integrated in the M^{c}DeLi code by replacing its d-Li reaction cross section and deuteron slowing down modules. The full package was then compiled with the MCNP4C routines [9], resulting in the advanced M^{c}DeLicious code which is capable of using evaluated data files for the neutron and photon generation through d-Li reactions.

It is worthwhile to note that an evaluation of neutron induced cross sections for the interaction with the lithium nuclides was provided by INPE too [7]. By making use of these data evaluations, it is possible to assess the neutron multiple scattering effect in the lithium target itself as well as the yield of secondary γ-rays due to the Li(n, xγ) reactions.

To check the data processing and sampling scheme of the d + ^{6,7}Li data by NJOY and M^{c}DeLicious, neutron and photon energy–angular distributions were calculated for a thin target consisting of either of the two lithium isotopes. The spectra for the particular deuteron energy were then converted to double-differential cross sections and compared with those derived directly from the ENDF formatted INPE file without any processing. Good agreement was found, validating thus the procedure applied with M^{c}DeLicious.

3. Comparison of M^{c}DeLicious, M^{c}DeLi and MCNPX results with experimental data

There have been a few independent measurements of neutron yield spectra from the deuteron bombardment of thick lithium targets [10–19]. To simulate these experiments we used a model adapted to a typical experimental configuration: a parallel mono-energetic beam of 1 cm diameter, a lithium target 4 cm in diameter and 4 cm thick, and a neutron detector recording the flux at 500 cm distance from the target. The problem of multiple neutron scattering effects on the target materials (lithium) was investigated by means of calculations with the newly developed M^{c}DeLicious code and n-Li data from INPE evaluations. It was shown that the neutron–lithium collisions inside the target resulting in neutron absorptions amount to 10–15% of the neutron flux and

should be therefore taken into account when comparing with experimental results.

Fig. 1 compares the experimental total and forward neutron yields with the M^{c}DeLi, M^{c}DeLicious and MCNPX calculations as a function of deuteron energy. Note that the experimental data were measured using different energy thresholds ranging from 0.3 to 3.5 MeV. Therefore, the related calculations were performed with a neutron energy threshold of 2 MeV. One can conclude that M^{c}DeLicious with the evaluated d-Li data from INPE predicts the energy dependent neutron yield better than M^{c}DeLi or MCNPX do. It is also seen that M^{c}DeLi is not capable of reproducing the experimental data below 20 MeV, whereas MCNPX underestimates the neutron yield by factor of 2.

The angular distributions of the emitted neutrons are shown in Fig. 2 for incident deuteron energies 15–40 MeV. For the deuteron energy 40 MeV, the three approaches considered in this work give results close to each other, which compare favourably to the experimental data. The MCNPX results, however, reveal a somewhat weaker anisotropy in the forward hemisphere,

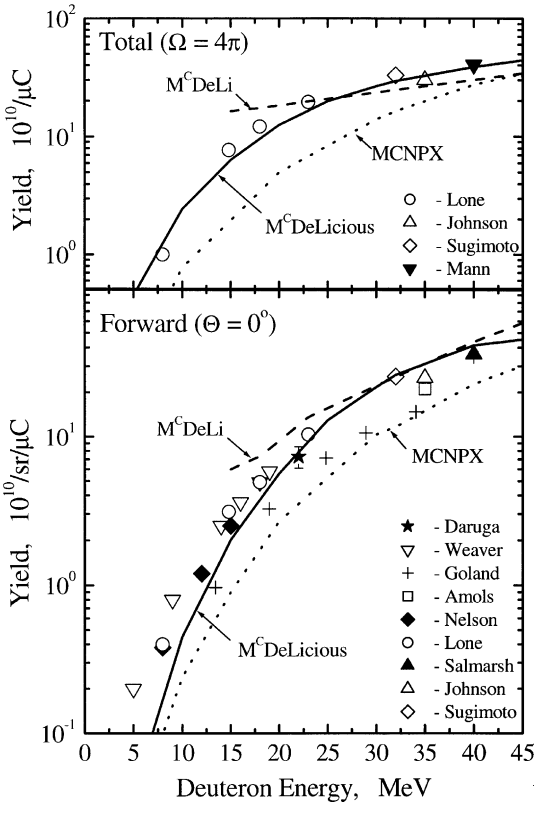

Fig. 1. Total (upper) and forward direction (bottom) neutron yields from thick lithium target versus bombarding deuteron energy. Symbols – experimental results [10–19], solid curves – M^{c}DeLicious, dashed – M^{c}DeLi, dotted – MCNPX.

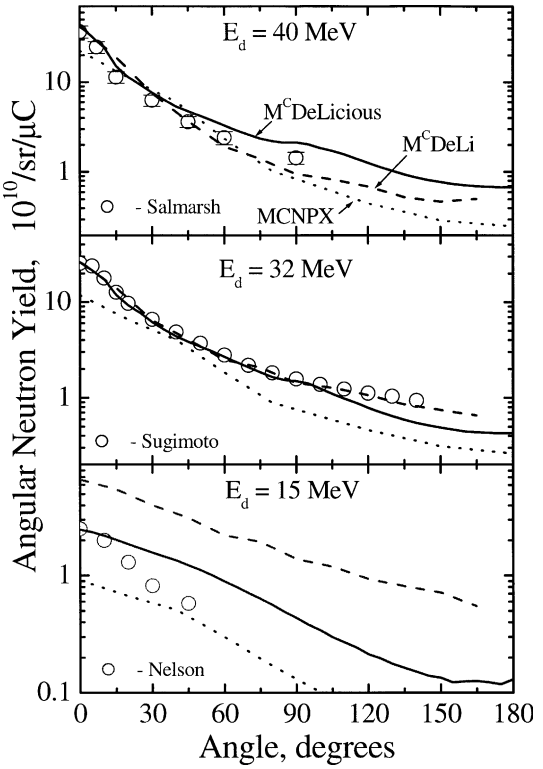

Fig. 2. Angular distribution of neutron yield from thick Li-target at different deuteron energies. Symbols – experimental results [14,16,18], solid curves – M^{c}DeLicious, dashed – M^{c}DeLi, dotted – MCNPX.

which is important for the IFMIF application. With decreasing incident deuteron energy the calculated spectra deviate more and more from each other and also disagree with the experimental results. At 15 MeV deuteron energy, only M^{c}DeLicious provides fairly good agreement with the measured data.

Double differential data – spectral neutron yields at different emission angles – are presented in Figs. 3 and 4 for the two deuteron energies 32 and 40 MeV. These figures again show that M^{c}DeLicious agrees better with experimental results than M^{c}DeLi and MCNPX, in particular. It is also revealed that a further essential improvement with the INPE data was achieved in the high energy part of the spectra ($E_n > 30$–40 MeV). These neutrons, produced in the exothermic ^{7}Li(d, n)^{8}Be reaction ($Q = 15$ MeV), were not taken into account in the M^{c}DeLi approach. The yield of these high energy neutrons is relatively small (≈0.5%), but they have significant importance for the activation and shielding behaviour.

The principal new possibility, which the updated code M^{c}DeLicious has opened, is the assessment of the γ-ray yield produced in the Li target. There are two physical processes which produce photons in the lithium

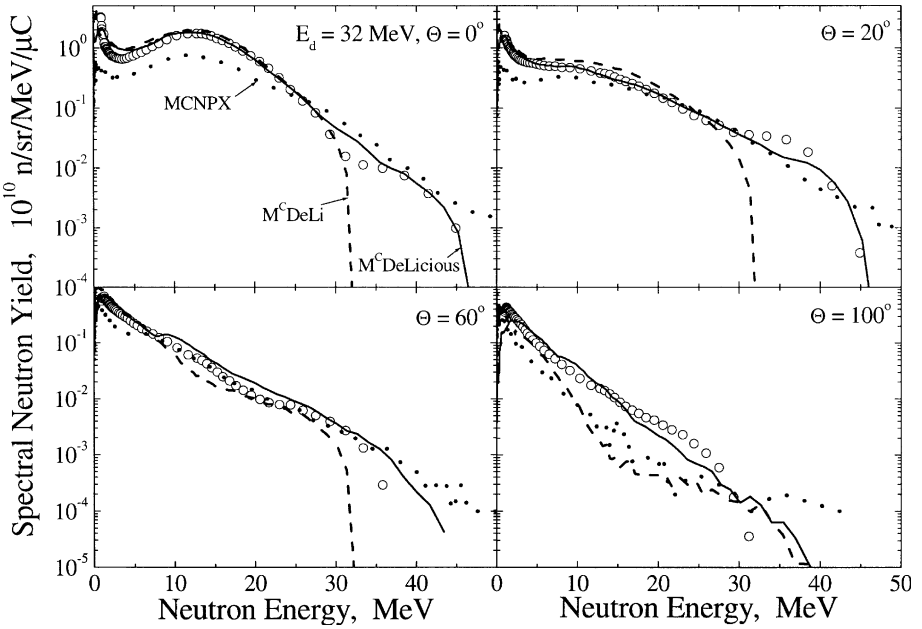

Fig. 3. Neutron energy spectra at different emission angles and deuteron energy 32 MeV. Symbols – experiment [18], solid curves – M^{c}DeLicious, dashed – M^{c}DeLi, dotted – MCNPX.

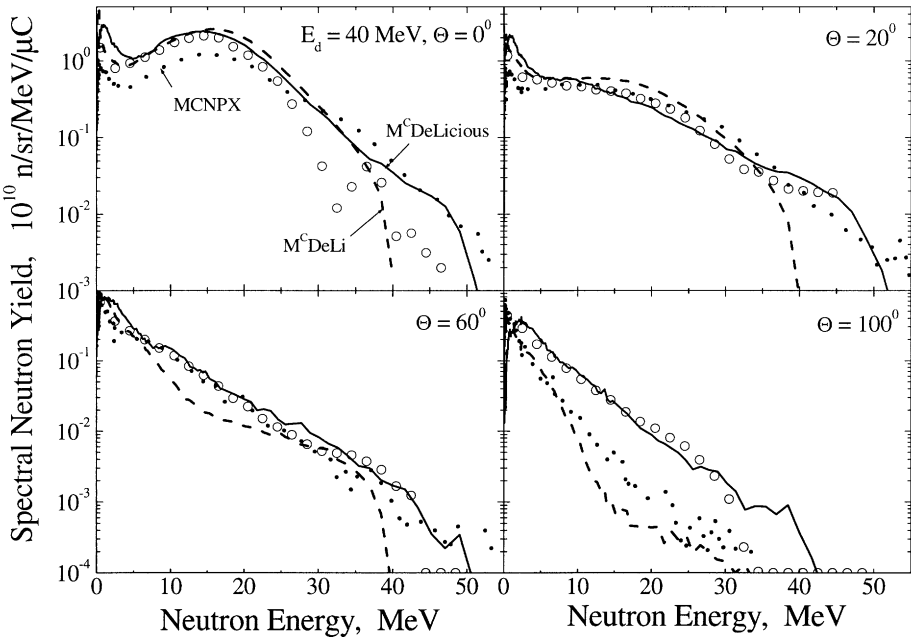

Fig. 4. Neutron energy spectra at different emission angles and deuteron energy 40 MeV. Symbols – experiment [19], solid curve – M^{c}DeLicious, dashed – M^{c}DeLi, dotted – MCNPX.

target: first, the primary reaction Li(d, xγ), and, second, neutron induced secondary reactions such as the inelastic scattering of source neutrons on lithium nuclei, i.e. the Li(n, xγ) reaction. Both of these production paths were analysed by means of M^{c}DeLicious calculations using the evaluated INPE data for d + ^{6,7}Li and n + ^{6,7}Li. The contribution of the neutron induced γ-ray production depends on the size and mass of the lithium

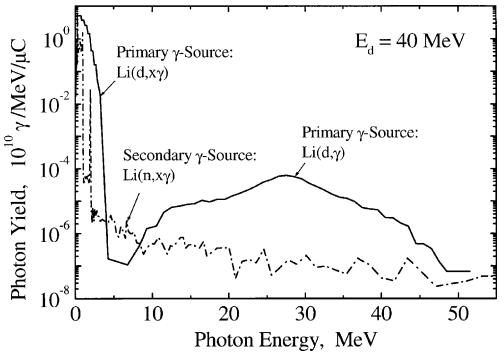

Fig. 5. Photon spectral yield from thick lithium target at deuteron energy 40 MeV. Results of M^{c}DeLicious calculations: solid curve – primary yield from Li(d, xγ) reaction, dashed – secondary yield from neutron inelastic scattering on Li target, i.e. Li(n, xγ) reaction.

target. For the Li target of the size mentioned above (cylinder $\varnothing$ 4 × 4 cm, Li density 0.51 g/cm^3), it amounts to ≈8% of the deuteron induced γ-ray yield, which, in turn, is one order of magnitude less than the total neutron yield. The photon energy spectra, depicted in Fig. 5, show that most of the γ-rays have energies below 5 MeV. Nevertheless, γ-rays with very high energies (10–50 MeV) are also produced in both deuteron and neutron capture reactions on the target nuclei. Although the fraction of such photons is relatively small (10^{-4}) they will result in nuclear transmutation and atomic displacement reactions in the IFMIF test modules, since their energies exceed the photo-nuclear reaction thresholds.

4. Conclusion

The advanced Monte Carlo code M^{c}DeLicious has been developed for enabling neutronics calculations for the d-Li based IFMIF neutron source, by making use of evaluated double-differential d + ^{6,7}Li cross section data. The comparison of calculated results with available measured data from thick lithium target deuteron experiments has shown that M^{c}DeLicious predicts the neutron yield spectra better than M^{c}DeLi or MCNPX do, both of which use built-in analytical models for the Li(d, xn) reaction cross section. The code M^{c}DeLicious is also capable of describing the photon production in the lithium target. With the new M^{c}DeLicious approach, further improvements of the d-Li neutron source term can be easily accomplished as soon as updated and validated d-Li data become available.

Acknowledgements

This work has been performed in the framework of the nuclear fusion programme of Forschungszentrum Karlsruhe and is supported by the European Union within the European Fusion Technology Programme.

References

[1] M. Martone (Ed.), IFMIF – International Facility Conceptual Design Activity – Final Report, ENEA Frascati Report RT/ERG/FUS/96/11, 1999.
[2] P.P.H. Wilson, Neutronics of the IFMIF neutron source: development and analysis, Forschungszentrum Karlsruhe Report FZKA 6218, 1999.
[3] J.F. Ziegler et al., The Stopping and Range of Ions in Solids, Pergamon, New York, 1985.
[4] J.F. Briesmeister (Ed.), MCNP – A General Monte Carlo N-Particle Transport Code, Version 4b, Los Alamos National Laboratory Report LA-12625-M, 1997.
[5] S.P. Simakov, Testing and updating of the M^{c}DeLi Monte Carlo Code, Forschungszentrum Karlsruhe Internal Report, 2000.
[6] L.S. Waters (Ed.), MCNPX^{TM} User's Manual, version 2.1.5, available from http://mcnpx.lanl.gov.
[7] A.Yu. Konobeev et al., Nucl. Sci. Eng. 139 (2001) 1.
[8] R.E. MacFarlane et al., NJOY99.00 – Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data, RSICC Code Package PSR-480, Oak Ridge, 1999.
[9] J.F. Briesmeister (Ed.), MCNP^{TM} – A General Monte Carlo N-Particle Transport Code, Version 4C, Los Alamos National Laboratory Report LA-13709-M, 2000.
[10] V.K. Daruga et al., Atomnaya Energiya 24 (1968) 71.
[11] K.A. Weaver et al., Nucl. Sci. Eng. 52 (1973) 35.
[12] A.N. Goland et al., IEEE Trans. Nucl. Sci. NS-22 (1975) 1776.
[13] H.I. Amols et al., Med. Phys. 4 (1977) 486.
[14] C.E. Nelson et al., Neutron spectra from deuteron and proton bombardment of thick lithium targets, Brookhaven National Laboratory Report BNL-NCS-50681, 1979.
[15] M.A. Lone et al., Nucl. Instrum. and Meth. 143 (1977) 331.
[16] M.J. Saltmarsh et al., Nucl. Instrum. and Meth. 145 (1977) 81.
[17] D.L. Johnson et al., J. Nucl. Mater. 85&86 (1979) 467.
[18] M. Sugimoto, private communication.
[19] F.M. Mann et al., Neutrons from d + Li and the FMIT irradiation environment, Hanford Engineering Development Laboratory Report HEDL-TC-1459, 1981.