

# Nuclear heating calculation for the high flux test module in IFMIF

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The PHITS code is applied to neutronics calculations for the high flux test module in IFMIF. The calculated neutron energy spectrum and heating rate show reasonably good agreement with the previous result of the conceptual nuclear design. These physical quantities are calculated using different high-energy nuclear data libraries (LA150, NRG-2003, and JENDL/HE-2004), and the similarities and differences are discussed. The validity of the KERMA approximation and the sensitivity of the Li(d,xn) neutron source term to heat production calculation are examined.

## 1. Introduction

The International Fusion Materials Irradiation Facility (IFMIF)<sup>1)</sup> is composed of an accelerator-driven deuteron-lithium neutron source for irradiation tests of fusion reactor candidate materials. Neutrons up to about 55 MeV will be produced by two 125 mA beams of 40 MeV deuterons bombarding a thick target of flowing liquid lithium. So far, conceptual nuclear designs of the IFMIF have been performed mainly using a code M<sup>c</sup>Delicious developed in Forschungszentrum Karlsruhe (FZK)<sup>2,3)</sup>. In detailed design of the IFMIF, more accurate estimation will be required on behaviors of fast neutrons with energies up to 55 MeV in materials. Several high-energy particle transport codes such as MCNPX<sup>4)</sup> and PHITS<sup>5)</sup> are widely used for various accelerator applications in combination with the latest high energy nuclear data libraries. Therefore, it is worthwhile to test to what extent these codes and high energy nuclear data libraries are applicable to IFMIF neutronics calculations.

The PHITS code<sup>5)</sup> is chosen for calculations of nuclear heating in the high flux test module (HFTM) in the IFMIF. The main purpose of this work is to examine the applicability of the PHITS code to IFMIF neutronics calculations. Neutron energy spectrum and nuclear heating over the HFTM are calculated and compared to FZK results. Furthermore, the sensitivity of three nuclear data libraries (LA150<sup>6)</sup>, NRG2003<sup>7)</sup>, and JENDL/HE-2004<sup>8)</sup>) to nuclear heating and the validity of KERMA approximation are discussed. Influence of the d-Li reaction source term is investigated on nuclear heating using differential thick target neutron yield data of the Li(d,n) reaction measured recently in Tohoku University<sup>9)</sup>.

## 2. Calculation procedure

The high flux test module (HFTM) is placed downstream behind the flowing liquid lithium target, forming the highest neutron radiation region. The HFTM consists of a steel container housing a number of irradiation rigs that contain encapsulated irradiation specimens.

The PHITS code is used for IFMIF-HFTM neutronics calculations. The details of the PHITS code are described in ref.<sup>5)</sup>.

In the present calculation, a simplified HFTM configuration is adopted as in the previous FZK work<sup>2)</sup>. The geometrical configuration is depicted in Fig.1. The HFTM part is composed of a rectangular block 20 x 5 x 5 cm<sup>3</sup> filled with Eurofer with a mass density of 6.24 g/cm<sup>3</sup>, which is 80% of the normal density to take account of the space occupied by cooling gas.

Each of two deuteron beams impinges on the lithium target with 10° declination angle in vertical direction. Fig.1 illustrates the lithium target (26 x 2.5 x 20 cm<sup>3</sup>) filled with lithium at 0.512 g/cm<sup>3</sup> and its back plate (26 x 0.18 x 20 cm<sup>3</sup>) filled with Eurofer at 7.8 g/cm<sup>3</sup> density. The PHITS code can calculate neutron production from the Li(d,xn) reaction in the lithium target using the QMD model<sup>10)</sup> in principle, but a preliminary result does not show reasonable agreement with experimental results. Thus, the differential thick target neutron yields (TTY) calculated by the M<sup>c</sup>Delicious code<sup>2)</sup> are used as the source term in the present work. The source term is assumed to be a surface source placed at a distance corresponding to the range of deuteron in lithium, although it is a volume source in practice. The tilt angles of ±10° of incident deuteron beam are taken into account so that the direction of neutron emission at 0° coincides with that of

the incident deuteron beam. It should be noted that scattering of neutrons from lithium layer between the surface neutron source and the back plate is neglected because the calculated TTY data are used as the neutron source term.

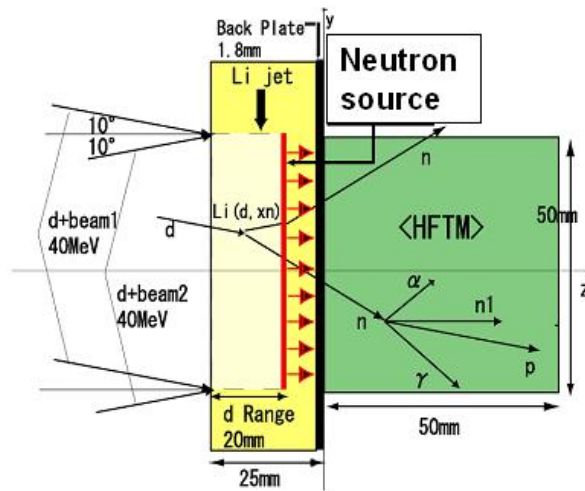


Fig.1 Geometrical configuration of the lithium target and HFTM

### 3. Results

#### 3.1 Applicability test of the PHITS code to IFMIF neutronics calculation

Energy distribution of the average neutron flux in the HFTM calculated by the PHITS code is compared with the FZK result obtained by the M<sup>c</sup>Delicious code<sup>2)</sup> in Fig.2. The former reproduces the latter well, although there is a slight difference in the energy range between 10 and 25 MeV. The difference might be due to that in the neutron source term, because the surface neutron source is assumed in the present work as mentioned in sect. 2. Table 1 shows comparisons of the average neutron and gamma fluxes, the average dpa rate, the total heat production, and the average heat production density. The present calculation shows agreement with the FZK result within about 10 %. Thus, this benchmark test indicates that the PHITS code is applicable to neutronics calculations for thermal-hydraulic design of the HFTM.

#### 3.2 Analysis of nuclear heating in the HFTM

The spatial distribution of nuclear heating rate in the HFTM is calculated for the case where each of two deuteron beams (2 x 125mA) impinges on the lithium target with 10° declination angle in horizontal direction. It should be noted that the beam incidence with horizontal declination is adopted in the latest IFMIF design<sup>3)</sup>. In fig.3, the result is presented as a three-dimensional plot sliced in half at x=0. The size of each boxel (i.e., an elementary cubic segment) is 0.5 x 0.5 x 0.5 cm<sup>3</sup>. The highest heating rate of 27 W/cm<sup>3</sup> is obtained in the vicinity of the surface region. The spatial distribution is also plotted along the depth into HFTM (i.e., z-axis) in Fig.4. It is found that the total heating rate is attenuated linearly with the depth and the dependence of neutron and gamma heating upon the depth is different.

Nuclear heating for other fusion reactor candidate materials (F82H, V4Ti4Cr, SUS304, and SiC) is also calculated in the same way using the PHITS code. For the sake of simplicity, the geometrical model used consists of a rectangular block 20 x 5 x 5 cm<sup>3</sup> filled with each material with the same mass density as the normal density, in order to see rough estimation of the dependence of nuclear heat production on materials. The result is shown in Table 2. The neutron and photo heat and their sum are almost same among three iron-based materials (Eurofer, F82H, and SUS304), while the total heat production for SiC, is much smaller than the other materials because the amount of photon heat released in the HFTM is considerably small.

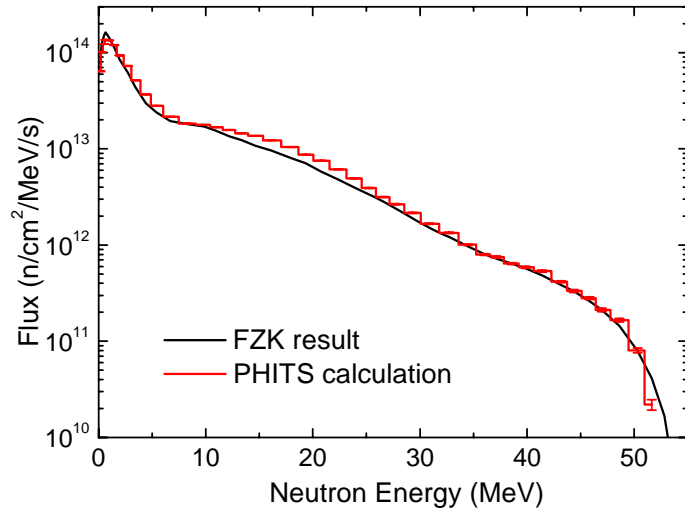


Fig.2. Comparison of neutron energy spectra in the HFTM between the present PHITS calculation and the FZK result<sup>2)</sup>

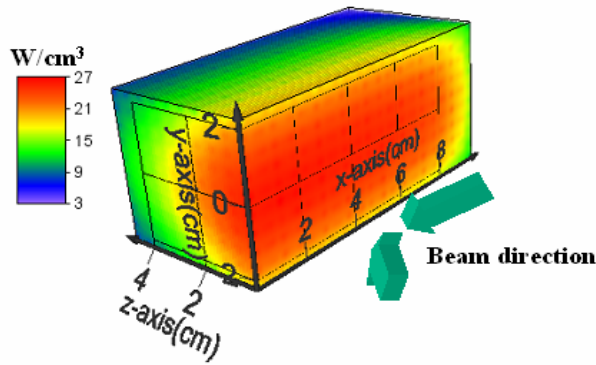


Fig.3. Three-dimensional spatial distribution of nuclear heating rate calculated by assuming deuteron beam incidence with horizontal declination

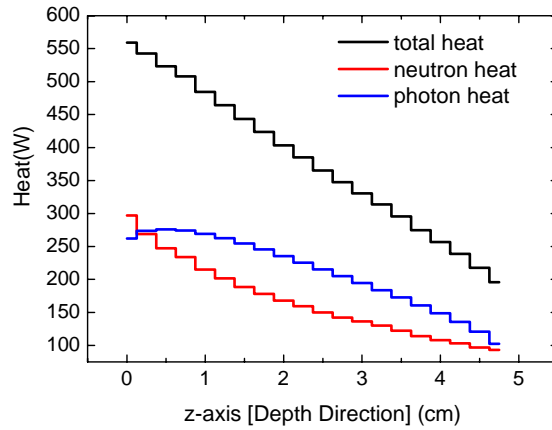


Fig.4. Spatial distribution of the heating rate produced in the HFTM along z-axis

Table 1. Physical parameters of the HFTM and results of neutronics calculations. The result of the FZK work is take from ref.<sup>2)</sup> for comparison.

Parameter	FZK work	Present work
Size	20 x 5 x 0.18 cm <sup>3</sup>	
Volume	500 cm <sup>3</sup>	
Material	Eurofer (Fe-88.9%, Cr-9.6%, C-4.9%, ...)	
Material Density	6.24 g/cm <sup>3</sup>	
Average Neutron Flux	5.86 x 10 <sup>14</sup> n/cm <sup>2</sup> /s	6.40 x 10 <sup>14</sup> n/cm <sup>2</sup> /s
Average Neutron Energy	7 MeV	7 MeV
Average Gamma-ray Flux	2.33 x 10 <sup>14</sup> γ/cm <sup>2</sup> /s	2.63 x 10 <sup>14</sup> γ/cm <sup>2</sup> /s
Average dpa rate	29 dpa/fpy	31 dpa/fpy
Total Heat Production	7.0 kW	7.5 kW
Average Heat Production Density	14 W/cm <sup>3</sup>	15 W/cm <sup>3</sup>

Table 2. Total heat production in the HFTM for different materials

material	Eurofer	F82H	V4Ti4Cr	SUS304	SiC
Total heating (kW)	9.94	9.50	9.70	10.70	6.10
Neutron (kW)	4.05	3.93	6.33	4.70	5.48
Photon (kW)	5.89	5.57	3.37	6.00	0.62

## 4. Discussion

### 4.1 Sensitivity of nuclear data library to calculation of nuclear heating and neutron flux

The neutronics calculations were performed using the PHITS code with three nuclear data libraries (LA150<sup>6)</sup>, NRG2003<sup>7)</sup>, and JENDL/HE-2004<sup>8)</sup>) in order to see how nuclear data libraries influence calculations of neutron flux and nuclear heating. As presented in Fig.5 and Table 3, the neutron fluxes are almost identical among three calculations, while the total heating rates are largely different (up to 50%). Table 3 indicates that the difference in the total heating rates is due to that in the heat generated by neutrons. This can be easily explained from the fact that the heating numbers of <sup>56</sup>Fe (i.e., kerma factors) included in the libraries are obviously different, particularly in the high energy range above 20 MeV, as seen in Fig.6.

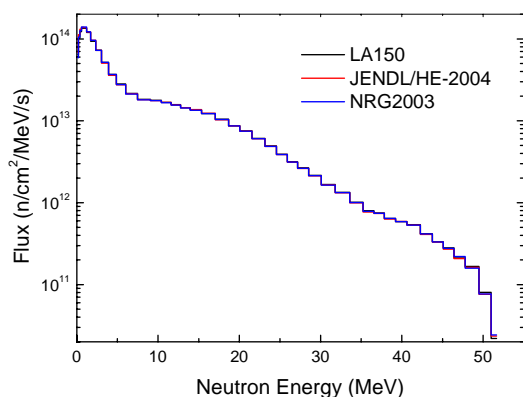


Fig.5. Comparison of the calculated neutron fluxes in the HFTM.

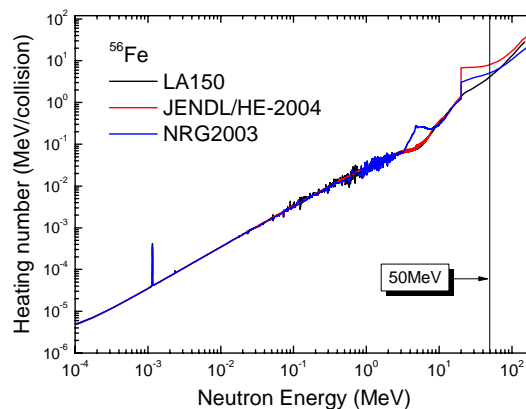


Fig.6. Total heating number of <sup>56</sup>Fe

Table 3. Comparison of calculated heating rates among three nuclear data libraries (LA150, JENDL/HE-2004, and NRG-2003)

Nuclear data library	LA150	JENDL/HE-2004	NRG-2003
Total heating rate (kW)	7.6	11.2	8.4
Neutron heating rate (kW)	3.4	6.7	4.4
Photo heating rate (kW)	4.2	4.5	4.0
Ratio to LA150	1	1.47	1.1

#### 4.2. Validity of KERMA approximation

As neutron energy increases, production of light ions, such as protons and deuterons with relatively high kinetic energy, becomes prominent. With an increase in the kinetic energy, the range becomes long, e.g., the range of 50 MeV protons is 5.3 mm in Eurofer with the mass density 6.24 g/cm<sup>3</sup>. Therefore, it is expected that the KERMA approximation assuming local energy deposition becomes worse. The PHITS code has a feature to deal with transport of light ions in matter using the continuous slowing down approximation. This means that the spatial spreading of the energy deposited by light ions can be taken into account beyond the KERMA approximation in the present calculation. It should be noted that the KERMA approximation is adopted for heavy recoils because the range is quite short. In the preceding work in FZK<sup>2)</sup>, the KERMA approximation was used in calculations of heat production. Therefore, it is of interest to examine quantitatively the validity of the KERMA approximation in the HFTM design.

The calculation condition is same as mentioned in sect. 2, except that neutrons enter in the direction perpendicular to the surface xy-plane of the HFTM. The PHITS calculation is implemented under the full KERMA approximation with the total heating numbers included in the nuclear data library, which is called the PHITS-KERMA calculation hereafter, and compared with the normal PHITS calculation mentioned in sect. 3. First, the total heat production is calculated by varying the depth along the neutron incident direction. The result is shown in Fig.7. Both the results are in good agreement for thickness over 1 mm. The KERMA approximation tends to overestimate because the light ions generated by neutron-induced reactions are likely to escape from the HFTM volume. Next, the neutron energy dependence is examined. In the calculation, mono-energetic neutrons impinge on the HFTM with different thicknesses of 1, 5, and 10 mm, respectively. Fig.8 presents the ratios of the total heat production calculated under the full KERMA approximation to the normal PHITS calculation. The ratios increase with increasing neutron energy and reducing thickness, and thus the KERMA approximation becomes worse and worse. Since the maximum energy of the source neutron in the IFMIF is about 55 MeV and the thickness of the HFTM is 25mm, however, the KERMA approximation is found to be valid in the heat production calculation in the HFTM. Finally, the spatial distributions of total heat production are compared between the two cases in Fig. 9. It is found that the difference appears slightly in the vicinity of the surface because most of generated light ions are expected to escape from the front surface.

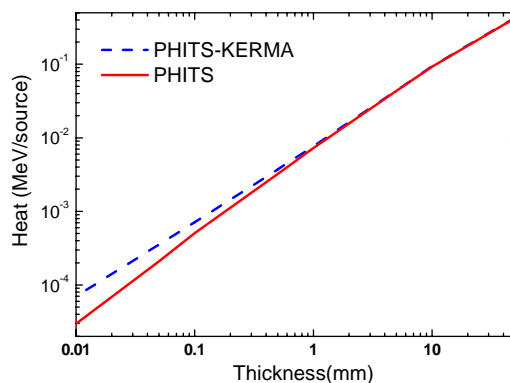


Fig. 7. Comparison of the total heat production between the full KERMA approximation and the normal PHITS calculation

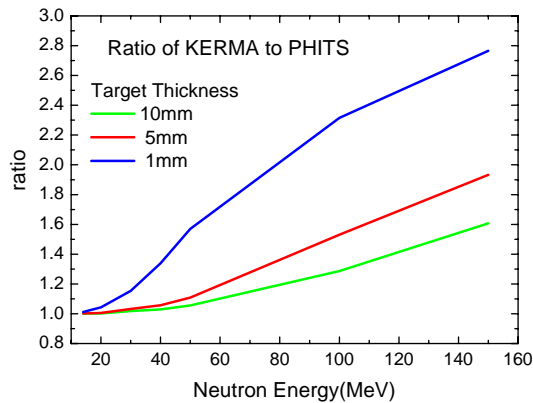


Fig.8. Ratio of the total heat production calculated under the full KERMA approximation to the normal PHITS calculation

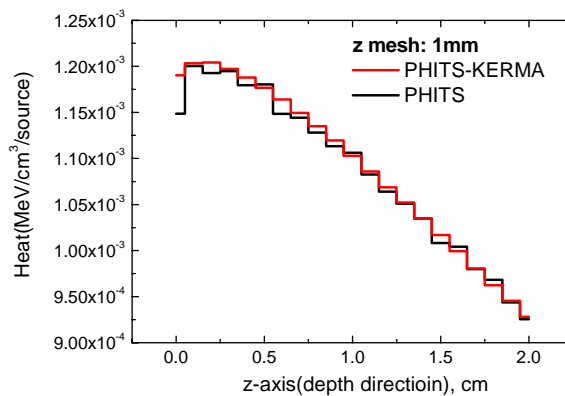


Fig. 9. Spatial distribution of total heat production

#### 4.3. Sensitivity of the d-Li neutron source

The M<sup>c</sup>Delicious neutron spectra used as input in the PHITS calculations mentioned early are compared with the recent experimental data of differential thick target neutron yields measured by Baba and co-workers<sup>9)</sup> in Fig.10. It is shown that the M<sup>c</sup>Delicious calculation overestimates the production of neutrons with energies below 5 MeV at 0° and the spectral shape is different from the observation at the high-energy end. Consequently, it is of interest to see how this difference affects the calculated neutron flux and heat production rate in the HFTM. In Fig.11, the PHITS result using the experimental data as the neutron source term is compared with that using the M<sup>c</sup>Delicious neutron spectra. There is no appreciable difference between the two calculations. However, it will be necessary to improve the overestimation seen in Fig.10 by re-evaluating the cross section data for the d + <sup>7</sup>Li reaction.

#### 5. Summary

The PHITS code was first applied to neutronics calculations for the high flux test module (HFTM) in the IFMIF neutron source facility. The calculated neutron energy spectrum and nuclear heating were in good agreement within 10% with the previous result by the FZK group. This indicates the applicability of the PHITS code to neutronics calculations for the HFTM. The calculation using different nuclear data libraries, LA150, NRG-2003, and JENDL/HE-2004, showed that the neutron fluxes are almost identical, while the heating rates have a large discrepancy, reflecting the difference in the heating numbers included in these libraries. In addition, it was confirmed that the KERMA approximation is reasonably good in calculating the heating rates in the HFTM unless one discusses the heat generated within the small size less

than 1 mm. Finally, the sensitivity of the  $\text{Li}(d,xn)$  neutron source term to nuclear heating in HFTM was examined, because there are some discrepancies between the  $M^c\text{Delicious}$  neutron spectra used in this work and the recent experimental data of differential thick target neutron yields. The heating calculation with the experimental data showed no remarkable difference from that with the  $M^c\text{Delicious}$  neutron spectra.

The PHITS code employs the quantum molecular dynamics (QMD) model<sup>10)</sup> to describe nuclear reactions that may take place in heavy-ion transport processes in matter. Its application to deuteron transport calculation is not necessarily successful. In addition, there are some discrepancies between the  $M^c\text{Delicious}$  calculation and experimental data as mentioned in sect. 4. Thus, we plan to study deuteron-induced reactions with particular focus on neutron production, aiming at further upgrading of IFMIF neutronics calculations.

Finally, our IFMIF-HTFM neutronics calculation will be linked with thermal-hydraulic design that is being performed by the Kyushu University group<sup>11,12)</sup> in the future.

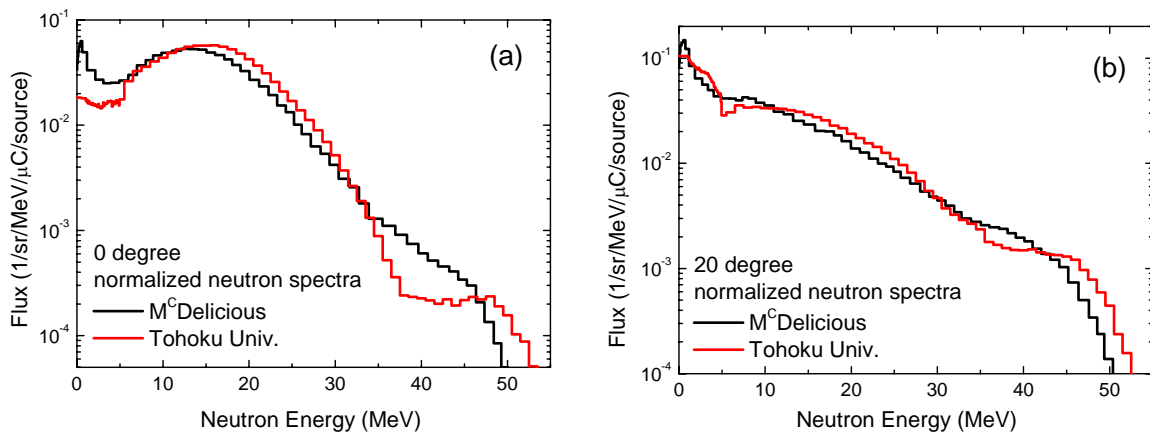


Fig. 10. Comparisons of calculated and measured thick target neutron yields from lithium at the deuteron incident energy of 40 MeV. The emission angles are 0 degree (a) and 20 degree (b), respectively. The experimental data are taken from ref.<sup>9)</sup>

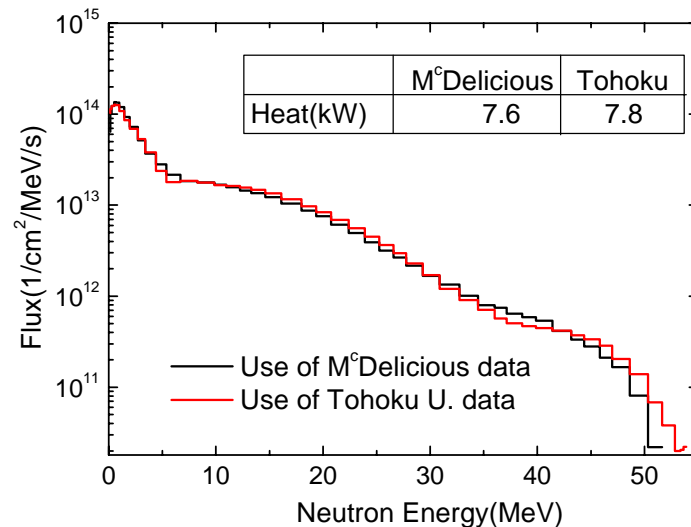


Fig.11. Comparison of average neutron fluxes and total heat production between the PHITS calculation with the  $M^c\text{Delicious}$  neutron source term<sup>2)</sup> and that with the experimental data<sup>9)</sup>

## Acknowledgements

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## References

- [1] H. Matsui, "Present status and future prospects of the IFMIF project", in Proceedings of the 23rd Symposium on Fusion Technology, Sept. 20-24, 2004, Venice, Italy.
- [2] S.P. Simakov, et al., "IFMIF neutron source term simulation and neutronics analysis of the high flux test module", Report FZKA 6743, Karlsruhe (2002).
- [3] U. Fischer, et al., Fusion Eng. Des. **81**, 1195-1202 (2006).
- [4] L.S. Waters(Ed.), MCNPX Users's Manual, Version 2.3.0, LA-UR-02-2607 (2002).
- [5] H. Iwasa, K. Niita, and T. Nakamura, J. Nucl. Sci. and Technol., **39**, 1142-1151 (2002).
- [6] M.B.Chadwick, et al., Los Alamos National Laboratory report LA-UR-99-1222 (1999).
- [7] A. J. Koning, et al., in Proceedings of the International Conference on Nuclear Data for Science and Technology, Santa Fe, USA, September 26-October 1, pp.422-425 (2004).
- [8] Y. Watanabe, et al., in Proceedings of the International Conference on Nuclear Data for Science and Technology, Santa Fe, USA, September 26-October 1, pp. 326-331 (2004).
- [9] M. Hagiwara et al., J. Fusion Sci. & Technol., **48**, 1320 (2005).
- [10] K. Niita, et al., Phys. Rev. C **52**, 2620 (1995).
- [11] S. Ebara, S. Nagata, H. Irida, T. Yokomine, and A. Shimizu, Fusion Eng. Des. **81**, 887-891 (2006).
- [12] S. Ebara, T. Yokomine, and A. Shimizu, Fusion Eng. Des. **82**, 61-72 (2007).