NUCL SCI TECH (2018) 29:140
https://doi.org/10.1007/s41365-018-0487-9

Preparation and verification of mixed high-energy neutron cross-section library for ADS

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Received: 1 December 2017 / Revised: 27 March 2018 / Accepted: 28 March 2018 / Published online: 29 August 2018

Abstract An accelerator-driven subcritical system (ADS) is driven by an external spallation neutron source, which is generated from a heavy metal spallation target to maintain stable operation of the subcritical core, where the energy of the spallation neutrons can reach several hundred mega-electron volts. However, the upper neutron energy limit of nuclear cross-section databases, which are widely used in critical reactor physics calculations, is generally 20 MeV. This is not suitable for simulating the transport of high-energy spallation neutrons in the ADS. We combine the Japanese JENDL-4.0/HE high-energy evaluation database and the ADS-HE and ADS 2.0 libraries from the International Atomic Energy Agency and process all the data files for nuclides with energies greater than 20 MeV. We use the continuous pointwise cross-section program NJOY2016 to generate the ACE-formatted cross-section data library IMPC-ADS at multiple temperature points. Using the IMPC-ADS library, we calculate 10 critical benchmarks of the International Criticality Safety Benchmark Evaluation Project manual, the 14-MeV fixed-source problem of the Godiva sphere, and the neutron flux of the ADS subcritical core by MCNPX. To verify the correctness of the IMPC-ADS, the results were compared with those calculated using the ENDF/B-VII.0 library. The results showed that the IMPC-ADS is reliable in effective multiplication factor and neutron flux calculations, and it can be applied to physical analysis of the ADS subcritical reactor core.

Keywords Accelerator-driven subcritical system · IMPC-ADS · MCNPX · NJOY2016 · Neutron cross section

1 Introduction

The nuclear data library is an indispensable element in reactor physics calculation and analysis. It contains relevant information about the cross section, decay data, and fission product share required by calculation programs. At present, there are five internationally recognized evaluation data libraries: the US evaluation library ENDF/B [1, 2], the European evaluation library JEF [3], the Russian evaluation library BROND [4], the Japanese evaluation library JENDL [5], and the Chinese evaluation library CENDL [6]. These databases are continuously updated, and ENDF/B is the most widely used. The evaluation libraries are based on existing experimental data and some reasonable interpolations or extrapolations using nuclear theoretical models. After evaluation and correction, the accuracy of the libraries can be confirmed. Finally, the evaluated libraries can be processed by cross-section programs such as NJOY [7], so that they can be used by Monte Carlo codes or deterministic codes. To date, most neutron evaluation libraries are designed for pressurized water reactors, and the upper limit of the neutron energy is generally 20 MeV, so they are not suitable for physics calculations of the accelerator-driven subcritical system (ADS) [8].

For the China Initiative Accelerator-Driven System (CIADS) [9], the designed energy of the proton accelerator

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This work was supported by the Strategic Priority Research Program of the Chinese Academy of Sciences (No. XDA03030102).

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is 250 MeV, and the neutron energy produced by the spallation target can reach over 200 MeV. Thus, existing databases can no longer meet the calculation requirements. At present, the nuclear data library used in ADS design is based mainly on the existing nuclear data library used in critical reactor design, with some improvements. These databases ignore the influence of neutrons with energies greater than 20 MeV, and this omission affects the accuracy of the calculation results [10].

With the development of accelerator-driven transmutation systems, as well as high-energy physics, ion beam applications, astrophysics, and research in space science, there has been a corresponding development of intermediate- and high-energy nuclear data worldwide, including JENDL/HE, LA150, and MENDL-2. The JENDL-4.0/HE library [11] is the most complete and contains 130 types of nuclides in the ENDF-6 format [12]. Here, the elastic scattering cross section and its angular distribution, particle generation cross section, and double-differential cross section are all based on experimental measurements and theoretical calculations. In the JENDL-4.0/HE library [11], the upper limit of the neutron energy is 200 MeV [13], but the library lacks evaluated cross-section files of some actinides, which are very important in ADS transmutation research.

An ADS-HE library [14] has been developed by Yavshits and Grudzevich to meet the requirements for transport calculations of high-energy neutrons. The evaluation data are from the ENDF/B-VII.1 [15], JENDL-4.0 [16], JEFF-3.1.2, and KRIT2n libraries. They include evaluated nuclear data files in the ENDF-6 and ACE formats for 10 fissionable nuclides, and the upper limit of the incident neutron energy is 1 GeV. The database is freely available from the International Atomic Energy Agency (IAEA) Nuclear Data Section. In 2008, the IAEA released the ADS 2.0 library [17]. The number of nuclides was increased from 30 to 156. However, only some of the nuclides have an upper energy limit of 150 or 200 MeV, so the above nuclear cross-section databases cannot meet the requirements for physics calculations of the CIADS.

In this paper, we select nuclides that have high-energy cross sections (above 20 MeV) from the JENDL-4.0/HE, ADS-HE, and ADS 2.0 libraries and process the ENDF-6-formatted files with the NJOY2016 [18] program to generate an ACE-formatted file at multiple temperature points. Thus, a new nuclear cross-section library, IMPC-ADS, was created for calculations for the ADS at the Institute of Modern Physics, Chinese Academy of Sciences. To verify its correctness, first, we used the MCNPX [19] program and chose 10 critical benchmarks from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) manual [20] to calculate the effective multiplication factor at different temperatures. Second, a 14-MeV fixed-source calculation for the Godiva critical sphere problem was performed. Third, for a reference design of the CIADS subcritical core, the flux distribution was calculated. Finally, we compared the results with those calculated using the ENDF/B-VII.0 [21] library in the three cases.

2 Program and method

2.1 Evaluated nuclear data source

The IMPC-ADS high-energy neutron cross-section library is used for reactor physics calculations of the CIADS device. It contains 139 nuclides, 122 of which came from the JENDL-4.0/HE library. The upper limit of the neutron energy is 200 MeV, and most structural materials in the subcritical reactor are included here. Further, some actinides such as ^{241}Am and ^{242}Am also appear; 10 nuclides are obtained from ADS-HE database, and the upper limit of the energy is 1 GeV. The remaining 7 nuclides are from the ADS 2.0 library; the upper energy limit of ^{233}U, ^{234}U, ^{236}U, ^{237}U, and ^{243}Am is 30 MeV, and that of ^{231} Pa and ^{233} Pa is 60 MeV.

The IMPC-ADS library is constructed using the NJOY2016 program. Considering the design and calculation requirements of the CIADS subcritical core, eight temperature points (293.6, 300, 600, 900, 1200, 1500, 1800, and 2100 K) are selected for each nuclide. The correspondence between the temperatures and the library indexes is shown in Table 1.

2.2 NJOY2016 parameter settings

NJOY is a widely used program developed by the Los Alamos National Laboratory for producing continuous pointwise cross sections and multigroup nuclear cross sections. The latest version is NJOY2016. It can process nuclide evaluation files in ENDF-6 format to generate multi-temperature ACE cross sections for reactor physics calculations. It consists of a set of subprocessing modules; the main modules used in producing the IMPC-ADS library are moder, reconr, broadr, heatr, gaspr, purr, thermr, and

Table 1 Correspondence between temperature and library index

Temperature (K)	Index	Temperature (K)	Index
293.6	02c	1200	12c
300	03c	1500	15c
600	06c	1800	18c
900	09c	2100	21c

acer. The essential processing parameters of NJOY2016 input files are shown in Table 2.

3 Verification of IMPC-ADS library

IMPC-ADS and ENDF/B-VII.0 were utilized with MCNPX to complete critical k_{eff} calculations of the ICSBEP benchmarks, the fixed-source calculation in the Godiva problem, and the flux calculation of the CIADS subcritical reactor. The results calculated using ENDF/B-VII.0 are a basic reference to test the correctness and reasonableness of the results calculated using IMPC-ADS.

3.1 ICSBEP critical benchmark calculation

The ICSBEP manual is published by the Organization for Economic Co-operation and Development-Nuclear Energy Agency and can be used to verify the correctness of neutron cross-section libraries for critical calculation and other applications. Ten benchmarks were selected from this manual. Criticality benchmarks are grouped into five major categories: ^{233}U critical assemblies, intermediate-enriched ^{235}U (IEU), highly enriched ^{235}U (HEU), ^{239}Pu assemblies, and mixed metal assemblies [22]. Two benchmarks of each type were chosen. A detailed description of the benchmarks is shown in Table 3.

Effective multiplication factor (k_{eff}) calculations at multiple temperature points were performed using the MCNPX program and the IMPC-ADS high-energy library. The results were compared with those calculated using MCNPX and ENDF/B-VII.0. Four temperatures were selected: 293.6, 600, 900, and 1200 K. The benchmark problems were calculated using a total of 400 cycles, 40 of which were inactive cycles, and 3000 particles were simulated for each cycle. Figure 1 shows the magnitude of the k_{eff} calculated at different temperatures. The benchmark values of the k_{eff} were real experimental values, and the results calculated by the IMPC-ADS and ENDF/B-VII.0 libraries were within the range of the experimental values. Further, the maximum differences between the magnitudes of the k_{eff} calculated using the IMPC-ADS and ENDF/B-VII.0 libraries were 0.11, 0.142, 0.263, and 0.209% for 293.6, 600, 900, and 1200 K, respectively, which are within the acceptable range (0.4%). Thus, the IMPC-ADS high-energy neutron cross-section library is reliable for k_{eff} calculations.

Table 2 Parameters of NJOY2016 input

Parameter	Description	Value
Err	Reconstruction tolerance (%)	0.1
Errthn	Fractional tolerance for thinning (%)	0.1
Thnmax	Max energy for broadening (MeV)	20
Nbin	Number of probability bins	20
Emax	Maximum energy for thermal treatment (eV)	4

3.2 14 MeV fixed neutron source calculation for Godiva problem

The geometric structure in the Godiva problem is a solid sphere with a radius of 8.7407 cm. The sphere is made of a mixture of ^{235}U and ^{238}U. The nuclear density of ^{235}U is 4.495832E22 atom*cm^{-3}. The nuclear density of ^{238}U is 3.017691E22 atom*cm^{-3} [23]. The temperature of the material is 293.6 K; a total of 400 cycles are used in the critical calculation, with 80 inactive cycles, and 5000 particles are simulated in each cycle. Table 4 shows the results calculated using the ENDF/B-VII.0 and IMPC-ADS libraries. The k_{eff} difference between the two libraries is 0.083%.

Moreover, a fixed-source calculation test of the Godiva sphere is also conducted, in which a 14-MeV neutron source is placed at the center of the sphere. The distribution of the normalized flux density for different energy groups is shown in Fig. 2. The distributions given by the ENDF/B-VII.0 and IMPC-ADS libraries are essentially the same. For energies below 0.001 MeV, the flux given by ENDF/B-VII.0 is slightly higher than that of the IMPC-ADS library. Note that the low-energy evaluated nuclear data files of ^{235}U and ^{238}U below 20 MeV in the IMPC-ADS library come from the ENDF/B-VII.1 library, and the difference in the evaluated files may lead to this result. Figure 3 shows the spatial distribution of the flux density in the Godiva sphere. The results calculated using the two libraries show distributions with the same shape. However, the flux calculated using IMPC-ADS is slightly higher than that calculated using ENDF/B-VII.0 in each energy interval. This is because of the different evaluation library. Thus, the IMPC-ADS library is reliable for fixed-source calculations of the Godiva problem.

3.3 Subcritical core of CIADS model

A reference design for the subcritical core of the CIADS is shown in Fig. 4. From the inside to the outside of the core, the target zone, lead bismuth assemblies, fuel assemblies, 316L dummy assemblies, and external lead bismuth assemblies are placed separately. The proton beam energy is 250 MeV, and the radius is 5 cm. The target material is iron–tungsten–nickel alloy, which has a density of 9.55 g/cm^3. The fissile material in fuel assembly 1 in Fig. 4 is UO$_2$ with an enrichment of 19.5% for ^{235}U, and assembly 2 is a transmutation assembly with minor actinide

Table 3 Description of criticality benchmarks

ICSBEP number	Abbreviation	Description
^{233}U-MET-FAST-001	23umt1	Bare metal sphere of ^{233}U
^{233}U-MET-FAST-003 Case 1	23umt3a	Normal uranium-reflected sphere of ^{233}U
IEU-MET-FAST-002	ieumt2	Normal uranium-reflected cylindrical disks of HEU
IEU-MET-FAST-003	ieumt3	Bare IEU sphere with 36% enrichment of ^{235}U
MIX-MET-FAST-001	mixmet1	HEU-reflected Pu sphere
MIX-MET-FAST-003	mixmet3	HEU-reflected Pu sphere
PU-MET-FAST-001	pumet1	Bare sphere of Pu with 4.5% atomic fraction of ^{240}Pu
PU-MET-FAST-002	pumet2	Bare sphere of Pu with 20% atomic fraction of ^{240}Pu
HEU-MET-FAST-001 Case a	umet1ss	Unreflected sphere of HEU
HEU-MET-FAST-003 Case 1	umet3a	Tuballoy-reflected sphere of HEU

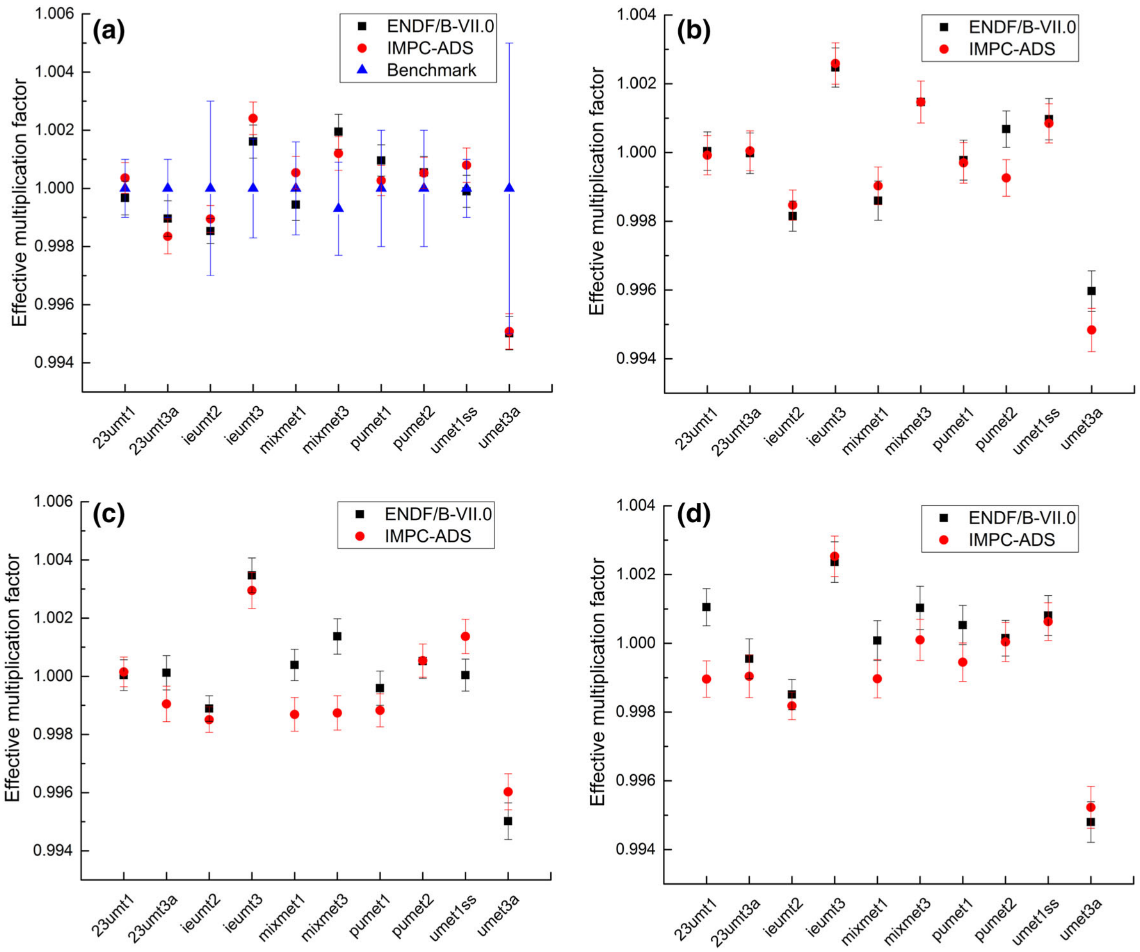

Fig. 1 K_{eff} at **a** 293.6 K, **b** 600 K, **c** 900 K, **d** 1200 K (Color online)

Table 4 k_{eff} result of Godiva critical sphere

Database library	k_{eff}	Relative standard error
ENDF/B-VII.0	0.99541	± 0.00047
IMPC-ADS	0.99624	± 0.00049

(MA) nuclides including ^{237}Np, ^{240}Pu, ^{241}Am, ^{243}Am. The total number of nuclides is 55, and they are all in the IMPC-ADS library. Therefore, k_{eff} and fixed-source calculations of the CIADS subcritical reactor are performed using the IMPC-ADS database to test whether it can be used in neutronics calculations of the CIADS. The reference k_{eff} values were obtained using the ENDF/B-VII.0 library. By combining the ENDF/B-VII.0 library for

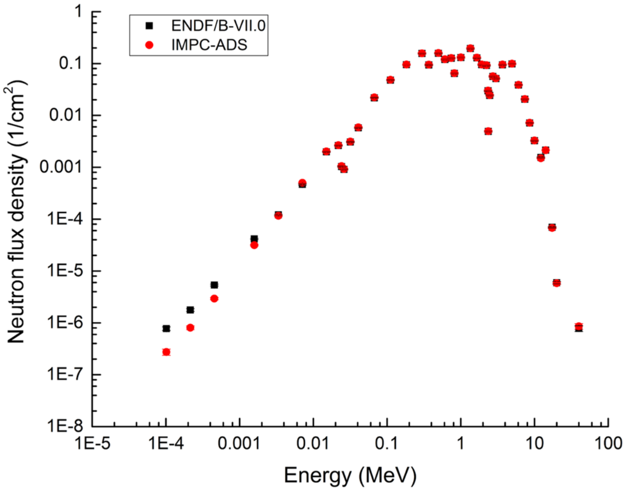

Fig. 2 Neutron flux density distribution for different energy groups (Color online)

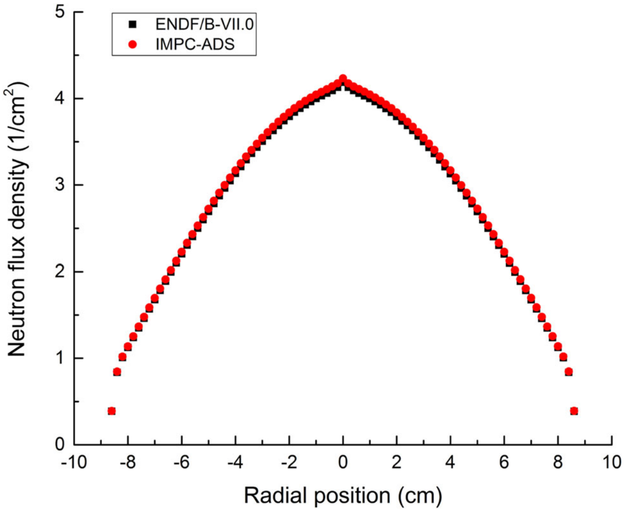

Fig. 3 Normalized neutron flux density distribution at various radial positions (Color online)

transport of neutrons below 20 MeV and a physical model of high-energy neutron transport, the reference result of the fixed-source calculation could be obtained via MCNPX using this combination.

3.3.1 Calculation of k_{eff}

In the calculation of the k_{eff}, each run of MCNPX has 30 inactive batches and 70 active batches, each with 5×10^4 particles. The critical neutron source is located at 40, 0, 0. Table 5 shows the k_{eff} values calculated using each data library. The difference in the k_{eff} value is 0.023%, which is within the normal range, so IMPC-ADS is reliable for k_{eff} calculation of the CIADS.

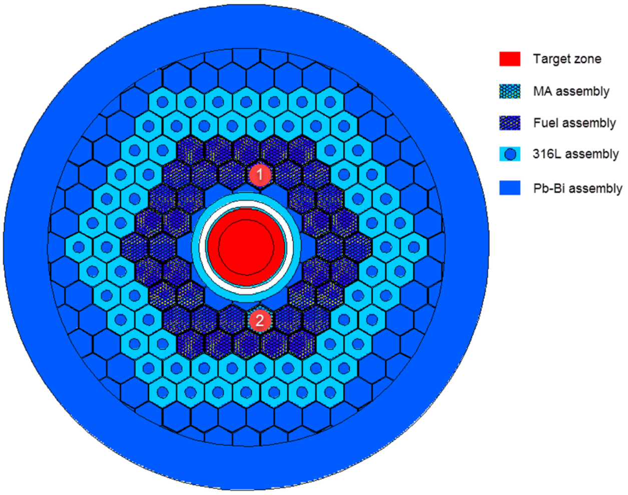

Fig. 4 Radial view of core region of CIADS (Color online)

Table 5 k_{eff} values obtained using different libraries

Database library	k_{eff}	Relative standard error
ENDF/B-VII.0	0.86268	± 0.00027
IMPC-ADS	0.86291	± 0.00028

3.3.2 Fixed-source calculation of core

To verify the correctness of the actinide cross-section data in the IMPC-ADS library, the flux distribution of the No. 1 fuel assembly and No. 2 MA assembly for 63 energy groups is calculated using the F4 card of MCNPX. By using F4 card in combination with the FS card, the axial distribution of the assembly flux from − 70 to 70 cm is also calculated.

The flux distributions in different energy groups within assembly No. 1 and No. 2 are shown in Fig. 5a, b, respectively. We can see that for the results calculated using IMPC-ADS and ENDF/B-VII.0, the neutron flux distributions show good agreement. Thus, the IMPC-ADS library gives a correct result for the flux distribution in different energy groups. Figure 6 shows the *Z*-axis flux distribution inside the assembly calculated using the FS card. The spatial flux distributions of assembly 1 and assembly 2 based on the two libraries are approximately the same. However, the total neutron flux values calculated using the IMPC-ADS high-energy library are approximately 5.79 and 4.42% higher than those calculated using the ENDF/B-VII.0 library for the MA and fuel assemblies. The reason is that the IMPC-ADS library has neutron cross-section library data at energies greater than 20 MeV. In the fixed calculation by MCNPX, transport of high-energy neutrons at energies greater than 20 MeV is realized

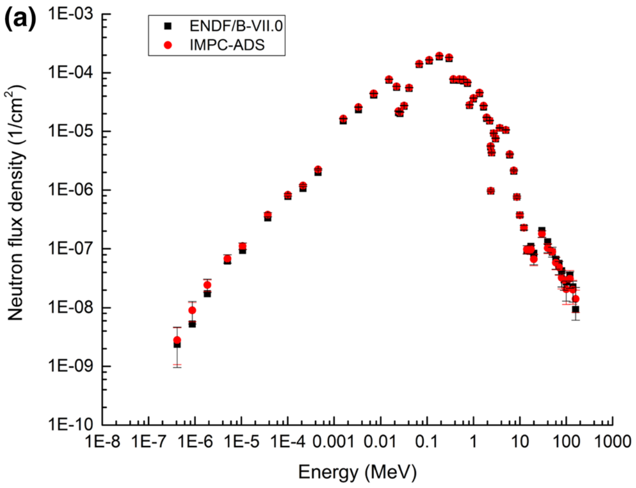

Fig. 5 Flux distribution in different energy groups for **a** fuel assembly (assembly 1), **b** MA assembly (assembly 2) (Color online)

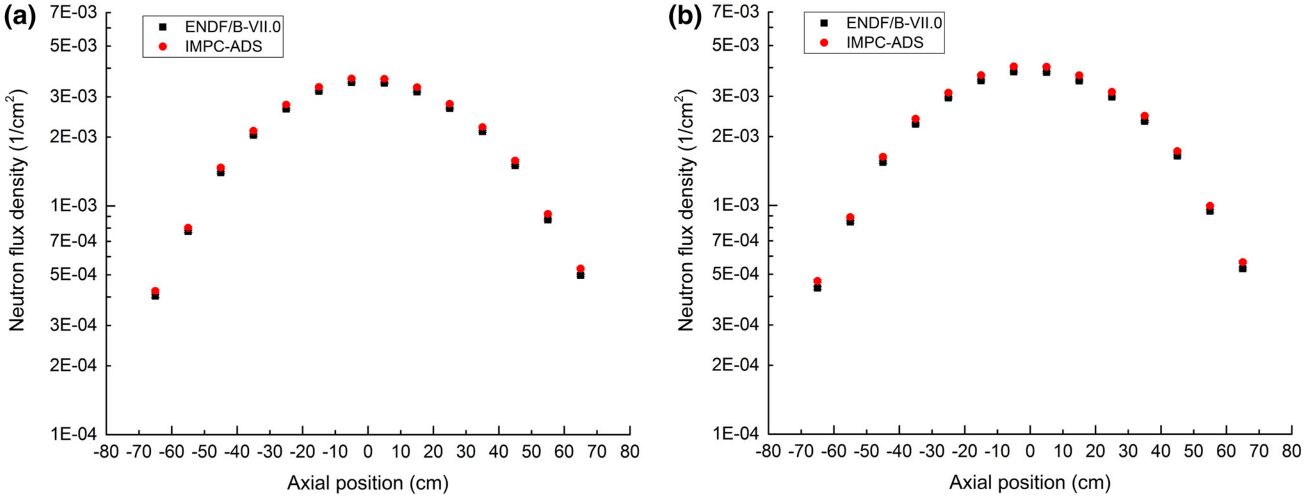

Fig. 6 Spatial distribution of flux at various assembly axial positions: **a** fuel assembly (assembly 1), **b** MA assembly (assembly 2) (Color online)

by using the fission cross section, scattering cross section, capture cross section, etc., within the IMPC-ADS library. Therefore, the high-energy neutrons and secondary fission reaction neutrons are considered in the MCNPX flux statistics. However, we should use the LCA and Phys:n cards to transport high-energy neutrons if the ENDF/B-VII.0 library is used because the upper energy limit of neutrons in the ENDF/B-VII.0 library is 20 MeV. Thus, by using the LCA and Phys:n cards, the CEM03 and LAQGSM physical model can be activated to transport high-energy neutrons. Then, a reference result can be obtained to test and verify the IMPC-ADS library. Thus, the flux difference in Fig. 6 results mainly from the difference caused by using the IMPC-ADS high-energy library and a physical model to transport high-energy neutrons.

The distribution of the neutron flux at different distances from the target zone in the *x* direction is calculated by mesh counting. The geometric division of the r-mesh cards is set as follows: The *x* direction extends from 24 to 100 cm at 2 cm intervals, the *y* direction extends from − 12 to 12 cm, and the *z* direction extends from − 10 to 10 cm. The result is shown in Fig. 7; the distributions of the normalized neutron flux calculated using the IMPC-ADS and ENDF/B-VII.0 libraries are in good agreement, but the flux at each position calculated using IMPC-ADS is greater than that calculated using ENDF/B-VII.0. The reason for this trend is that ENDF/B-VII.0 has no cross-section data for neutrons with energies greater than 20 MeV, and physical models are used to simulate the transport of high-energy neutrons; this process causes secondary fission. From the perspective of verifying the correctness of the library, the IMPC-ADS library can give a similar result close to that of the physical model, which basically proves the reliability of the library. Thus, application of the IMPC-ADS data

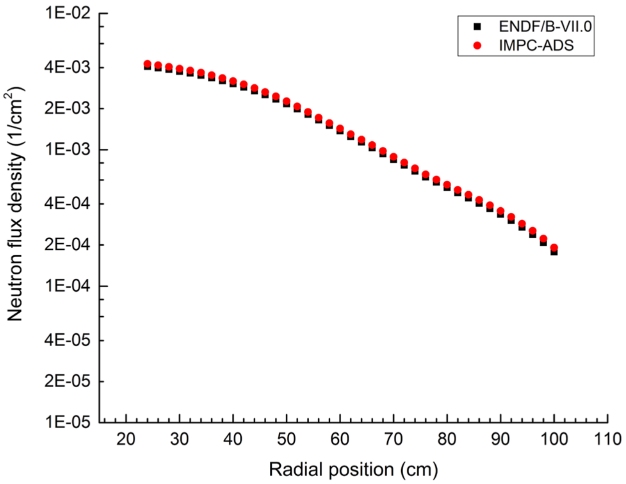

Fig. 7 Neutron flux density distribution in *x* direction in CIADS (Color online)

library in physical calculations of the CIADS reactor has been preliminarily verified.

4 Conclusion

This paper integrates the JENDL-4.0/HE, ADS-HE, and ADS 2.0 databases to create a mixed high-energy library, IMPC-ADS, so the effect of high-energy neutrons can be considered. The NJOY2016 program was used to generate ACE-formatted cross sections for reactor physics calculations of the ADS. Verification calculations of the IMPC-ADS library were carried out using the MCNPX program. The effective multiplication factor of ICSBEP benchmarks, the neutron flux distribution of the Godiva sphere, and CIADS subcritical core results are compared with the corresponding results calculated using the ENDF/B-VII.0 library. The physical model card is used for transport of high-energy neutrons, whereas the flux calculation is performed using ENDF/B-VII.0.

The results showed that the maximum difference between the effective multiplication factors of the ICSBEP benchmarks calculated using IMPC-ADS and ENDF/B-VII.0 is approximately 0.263%, which is within the normal range. The calculated neutron flux distributions are in good agreement. It was proven that the IMPC-ADS library is suitable and reliable for physics calculations and analysis of the ADS.

Because the IMPC-ADS library contains only 139 nuclides for the CIADS calculation, it may not include nuclides that are newly produced in the operation of the subcritical core. Thus, we need to integrate other cross-section evaluation libraries to develop the IMPC-ADS mixed high-energy library. Moreover, the IMPC-ADS library should also be applied to the code for burn-up calculations of the CIADS in the future.

Acknowledgements The authors acknowledge IAEA Nuclear Data Services for providing the ENDF-6 source files of all nuclides.

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