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Development of a 1200 fine group nuclear data library for advanced nuclear systems

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Abstract Accurate and reliable nuclear data libraries are essential for calculation and design of advanced nuclear systems. A 1200 fine group nuclear data library Hybrid Evaluated Nuclear Data Library/Fine Group (HENDL/FG) with neutrons of up to 150 MeV has been developed to improve the accuracy of neutronics calculations and analysis. Corrections of Doppler, resonance self-shielding, and thermal upscatter effects were done for HENDL/FG. Shielding and critical safety benchmarks were performed to test the accuracy and reliability of the library. The discrepancy between calculated and measured nuclear parameters fell into a reasonable range.

Keywords Advanced nuclear system · Fine group nuclear data library · Effective multiplication factor

1 Introduction

Advanced nuclear systems, such as fusion-driven subcritical and accelerator-driven subcritical systems, have been proposed to solve fuel breeding and waste transmutation for development of nuclear power. Nuclear data libraries with high accuracy and reliability are of importance for design and calculation of advanced nuclear systems.

A fine group or ultra-fine group nuclear data library contains thousands or ten thousands of energy groups, respectively, [1–3]. The structure of a fine group nuclear data library can ensure the accuracy of group approximation, while the coarse group collapsed from fine group nuclear data library can save calculation time and ensure enough precision.

Four sublibraries of Hybrid Evaluated Nuclear Data Library (HENDL) [4, 5] were developed by FDS Team [6–11]: the HENDL/MC is a point-wise data library; the HENDL/MG is a multi-group library with 175 neutron/42 gamma energy group structure; the HENDL/CG is a coarse-group library with 27 neutron/21 gamma energy group structure, and the hybrid evaluated nuclear data library/fine group (HENDL/FG) has 1200 neutron/42 gamma energy groups ($\leq$150 MeV).

In this paper, we report the design of HENDL/FG, and the shielding and critical safety benchmarks performed using SuperMC [12–17] to test its accuracy and reliability.

2 Design of HENDL/FG

HENDL/FG includes 320 nuclide cross-section files, covering moderators, structural materials, fission products, and actinides. The format of the cross-section files is MATXS. HENDL/FG was generated from ENDF/B-VII.1 and JEFF3.2 with NJOY code [18]. The design includes energy group structure, weight function and physical effect corrections.

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Table 1 Calculated and measured k_{eff} of spherical shells

Critical spheres	HENDL/FG 1200 groups	Collapsed group 72 groups	Measured
^{233}U-MET-FAST-1	0.99966	0.99799	1.0000
^{233}U-MET-FAST-2	1.00347	0.99434	1.0000
HEU-MET-FAST-1	0.99805	0.99788	1.0000
^{233}U-MET-FAST-4	1.00333	1.00441	1.0000
PU-MET-FAST-1	0.99903	0.99598	1.0000
PU-MET-FAST-5	1.00583	1.00726	1.0000
SPEC-MET-FAST-8	1.00024	0.99667	1.0000
SPEC-MET-FAST-1	0.99976	1.00258	1.0000
^{233}U-SOL-THERM-1	1.00043	1.00989	1.0000
PU-SOL-THERM-002-1	1.00310	1.00420	1.0000
^{233}U-SOL-THERM-001-1	1.00240	1.00340	1.0005

2.1 Energy group structure

The neutron energy structure of HENDL/FG is 1200 groups ranging from 10^{-5} eV to 150 MeV, and 54 neutron groups are above 20 MeV. The design of neutron energy of >20 MeV group structure were implemented by comprehensive analysis. The GNASH [19] code based on statistical hauser-feshbach plus pre-equilibrium exciton models was used to analyze the interaction between intermediate energy neutrons (<150 to 250 MeV) and the subcritical cladding materials. The nuclear reaction thresholds of new reaction channel between intermediate energy neutrons and nuclides were obtained. The neutron energy group bounds from 20 to 150 MeV were designed for HENDL/FG.

The neutron group structure from 10^{-5} to 4.0 eV is a detailed thermal structure of 80 groups. The neutron structure from 4.0 eV to 12.52 MeV is 1055 groups with a lethargy width of about 0.016, which corresponds to twice of the average lethargy increase by elastic scattering of ^{238}U. The neutron structure from 12.52 to 20 MeV is 11 groups according to Vitamin-J [18] group structure. The rest of the energy range is divided into 54 groups.

The gamma group structure is a typical group structure Vitamin-E [18] from 1 keV to 50 MeV.

The energy group structure of HENDL/FG can satisfy the requirement of nuclear design for advanced nuclear systems.

2.2 Weight function

The neutron weight functions of HENDL/FG are follows: a 0.0253-eV thermal Maxwellian below 4 eV, a l/*E* law for 4 eV–2.12 MeV, a 1.415-MeV fission spectrum for 2.12–10 MeV, another l/*E* section for 10–12.52 MeV, a fusion peak for 12.52–15.68 MeV, a final l/*E* section for 15.5–20 MeV, and an adopted 1/*E* spectrum for 20–150 MeV according to optimization analysis for advanced systems. The gamma weight function is 1/*E* + roll-offs [18] for 1 keV–50 MeV.

2.3 Corrections of physical effect

The corrections of Doppler effect [18], resonance self-shielding effect, and thermal up-scatter effect were considered in HENDL/FG. For Doppler effect, BROND [18] module was used to correct cross section at different temperatures. In this paper, 10 temperature ranges (296, 400, 500, 600, 700, 800, 1000 K, 1200, 1600, and 2000 K) are given in HENDL/FG. THERMR [16] module was used to correct thermal up-scatter effect. The scattering laws include ^{1}H: S(α,β) for hydrogen bound in water, ^{2}H: S(α,β) for deuterium bound in heavy water, ^{12}C: S(α,β) for carbon in graphite, and free gas model for all materials.

Bondarenko [18] and flux calculators [18] were used in correcting resonance self-shielding effects. For actinides, NJOY flux calculator and Bondarenko method were used for homogenous mixtures. Narrow resonance approximation was used for other materials. The correction of resonance self-shielding effect was implemented by making multi-group cross-section data library with different reference background cross sections. The precision of correction self-shielding effect was determined by selecting the background cross sections [4] in the design of HENDL/FG. For the nuclides in HENDL/FG, 10 reference background cross sections were chosen according to the compositions which the nuclides likely to be used. Typical design for advanced systems was considered in selecting the background cross sections. In this paper, the reference background cross sections (*barns*) are:

^{241}Am: 10^{10}, 10^{4}, 10^{3}, 500, 100, 50, 30, 10, 1, 0.1;
^{237}Np: 10^{10}, 10^{4}, 10^{3}, 500, 100, 50, 40, 10, 1, 0.1;
^{238}U: 10^{10}, 10^{4}, 10^{3}, 100, 50, 10, 1, 0.5, 0.3, 0.1.

Table 2 Results of neutron leakage rate

Sphere shell	Energy (MeV)	Experiment data (1/sn)	C/E (SuperMC)		Sphere shell	Energy (MeV)	Experiment data (1/sn)	C/E (SuperMC)	
			HENDL/FG	ENDF-B/VII.1				HENDL/FG	ENDF-B/VII.1
Be	0.003–1	0.469	1.041	1.022	Cu	5–10	0.013	1.217	1.329
	1–5	0.315	0.871	0.851		10–20	0.079	0.897	1.078
	5–10	0.143	1.012	0.942		0.1–20	0.898	0.986	1.058
	10–20	0.324	1.341	1.361	Zr	0.1–1	0.442	1.111	1.077
	0.003–20	1.260	1.072	1.051		1–5	0.307	1.078	1.106
Al	0.1–1	0.069	0.862	0.811		5–10	0.033	0.816	0.883
	1–5	0.148	0.912	0.923		10–20	0.317	1.306	1.381
	5–10	0.050	0.851	0.863		0.1–20	1.100	1.146	1.183
	10–20	0.675	1.111	1.163	Nb	0.1–1	0.335	1.195	1.084
	0.1–20	0.942	0.991	1.013		1–5	0.219	1.187	1.165
V	0.1–1	0.391	1.115	1.037		5–10	0.036	1.006	0.932
	1–5	0.301	1.094	1.131		10–20	0.510	1.076	1.132
	5–10	0.037	0.929	0.935		0.1–20	1.100	1.194	1.195
	10–20	0.381	0.912	0.979	Mo	0.1–1	0.516	0.871	0.839
	0.1–20	1.110	1.032	1.037		1–5	0.287	0.843	0.836
Cr	0.1–1	0.211	1.071	0.965		5–10	0.043	0.752	0.787
	1–5	0.221	1.091	1.025		10–20	0.524	0.989	1.033
	5–10	0.041	1.142	1.029		0.1–20	1.370	0.907	0.909
	10–20	0.549	0.942	1.043	W	0.1–1	0.360	1.131	0.931
	0.1–20	1.020	1.011	1.023		1–5	0.241	0.722	0.778
Fe	0.05–1	0.099	1.108	1.042		5–10	0.040	0.863	0.878
	1–5	0.140	1.141	1.035		10–20	0.710	1.026	1.022
	5–10	0.032	1.123	0.998		0.1–20	1.350	0.985	0.906
	10–20	0.740	0.975	1.018	Pb	0.4–0.8	0.173	1.059	0.967
	0.1–20	1.010	1.015	1.026		0.8–1.4	0.212	1.122	1.029
Co	0.1–1	0.242	0.986	0.907		1.4–2.5	0.231	1.198	1.091
	1–5	0.295	0.827	0.888		2.5–4	0.100	1.096	1.083
	5–10	0.055	0.926	0.956		4–6.5	0.035	1.066	0.992
	10–20	0.729	1.031	1.074		6.5–10.5	0.038	0.644	0.615
	0.1–20	1.320	0.931	0.928		10.5–20	0.488	0.967	1.061
Cu	0.1–1	0.660	0.998	1.061		0.4–20	1.280	1.051	1.033
	1–5	0.145	0.957	1.029					

3 Benchmark results and discussion

Shielding and critical safety benchmarks were performed using SuperMC to test the accuracy and reliability of HENDL/FG.

3.1 Critical safety benchmark

The critical spheres were derived from International Criticality Safety Benchmark Evaluation Project [20]. The calculated k_{eff} results are given in Table 1, agreeing well with the measurement data (within 0.5%). The k_{eff} was calculated, too, by 72 groups data library collapsed from HENDL/FG. The groups in neutron energy of up to 10 MeV were collapsed into one group, while the groups under 10 MeV were collapsed into 71 groups according to near structure of WIMSD-69 group. Therefore, a mesh structure of 72 groups was produced.

3.2 Shielding benchmark with 14 MeV neutron

The shielding integral experiments [21–23] were based on sphere shell geometry with a 14 MeV D-T fusion neutron source at the center of the inner void sphere. The simulation results of C/E values of integral neutron leakage rate from SuperMC & HENDL/FG and SuperMC & ENDF/B-VII.1, and the corresponding experimental measured values are listed in Table 2. ENDF/B-VII.1 is a

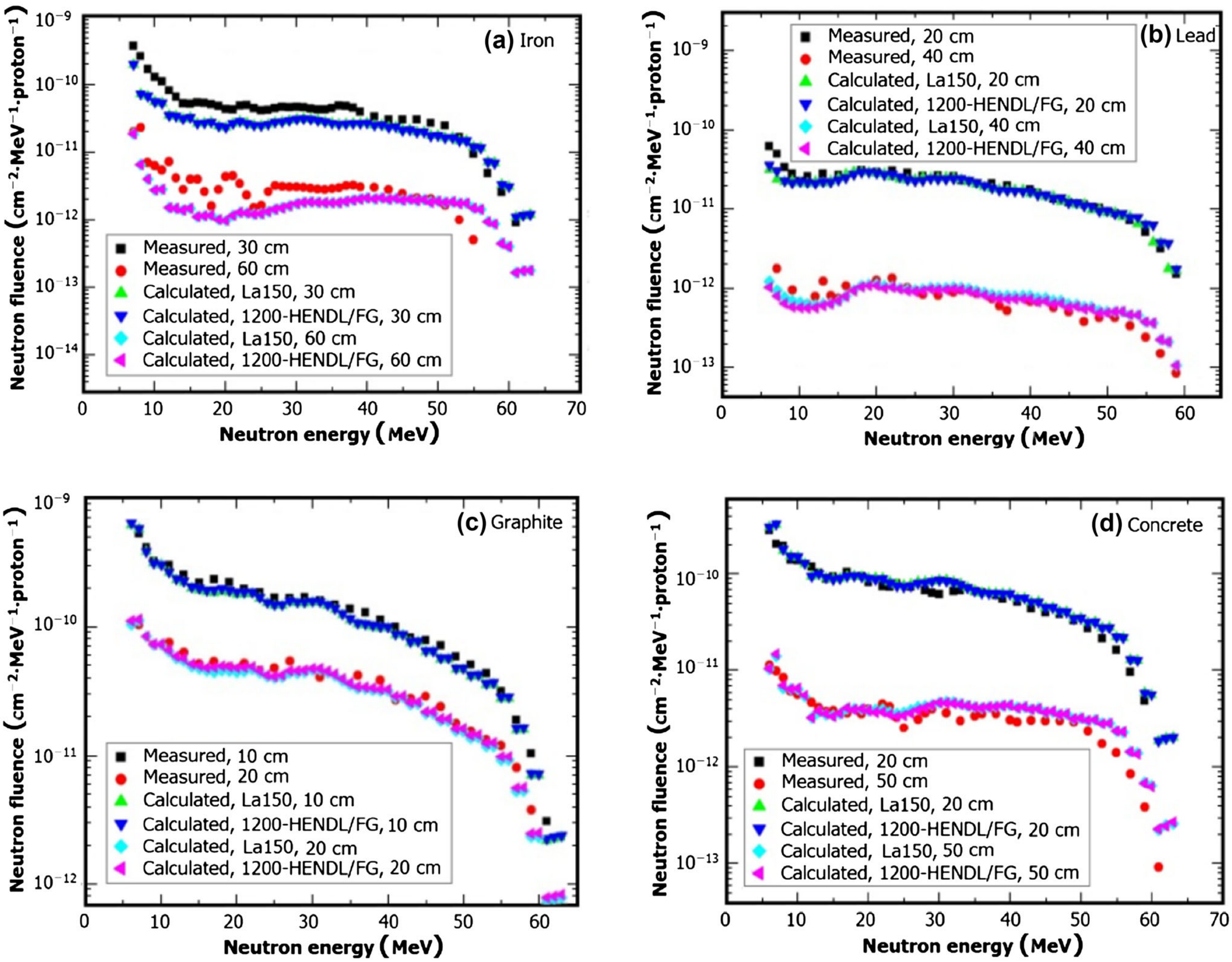

Fig. 1 Experiment benchmark of **a** iron, **b** lead, **c** graphite and **d** concrete shieldings

point-wise ACE format data library processed by ENDF/B-VII.1 evaluated data file.

For Be, V, Co, Mo, and Zr spherical shells, the neutron leakage spectra calculated by HENDL/FG and ENDF/B-VII.1 calculations agree well with the experiment results, with the differences being less than 10%; while they become larger than 10% for the spherical shell of Al, W, Si, Ti, Cr, Fe, Cu, Nb, and Pb spherical shells. In some energy ranges, for Be, Si, Ti, Cu, Zr, Nb, Mo, W, and Pb, the HENDL/FG calculation results differ greatly from the experimental data, while the differences are even bigger for Al and Co. These may be caused by the error of evaluation source data and experimental data itself.

3.3 Shielding Benchmark with TIARA in AVF

To validate and qualify the cross section of neutrons in energy of >20 MeV for HENDL/FG library, the neutronics integral experiments—TIARA (JAERI) [24] on AVF cyclotron at Osaka University, were performed by SuperMC& HENDL/FG.

In these experiments, copper target were bombarded by protons to produce secondary neutrons and protons. The secondary neutrons were captured by NE213 detectors on the beam axis and at 5–7 cm off the beam axis behind the test shieldings of iron, lead, graphite, and concrete in different thicknesses.

The measurements for neutron spectra above 10 MeV on the beam axis were carried out; while Monte Carlo calculations with MCNPX [25] code and LA150 [26] data library were performed for the benchmark analyses. The results are compared with those of HENDL/FG, as shown in Fig. 1.

From TIARA neutron flux benchmark experiments, one sees that calculation results of HENDL/FG are good for small thicknesses of the shieldings, whereas for the shielding layer thickness of 50–60 cm, the difference between the calculation and experiment results increases. For the Fe and Pb benchmark experiments, the difference of neutron flux between HENDL/FG and experiment exceeds 22%. The calculations with HENDL/FG are almost the same as MCNPX and LA150 calculations for these models, and the difference was about 7% between HENDL/FG with LA150 nuclear data library.

4 Conclusion

In this paper, a 1200 fine group nuclear data library HENDL/FG for neutron energy up to 150 MeV based on ENDF/B-VII.1 and JEFF3.2, is developed, which considers complex physical effects in the nuclear analysis for advanced nuclear systems.

The shielding and critical safety benchmarks were performed to validate the cross section for neutron energy of >20 MeV for HENDL/FG library, and the transport calculations for TIARA neutronics integral experiments. The results indicate that the discrepancy between calculation and experimental values of nuclear parameters fell into a reasonable range.

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