

Validation of CENDL-2.1 and Progress on CENDL-3

Liu Tingjin

(Chinese Nuclear Data Center)

Since last NEA WP meeting in June, 1995, considerable progress on CENDL project has been made. Following are the main points.

1. Validation and Improvement of CENDL-2.1

A modified version of CENDL-2, i. e. CENDL-2.1 was completed and released in the end of 1995^[1]. The library contains complete neutron data of 68 nuclides (elements) from ^1H to ^{249}Cf in the neutron range from 10^{-5} eV to 20 MeV.

Compared to CENDL-2, the data have been increased, modified and improved significantly :

	Nuclides	MF6	MF12-15	MF31-33
CENDL-2	58	4	10	7
CENDL-2.1	68	25	38	10
increment	14	21	28	3

In CENDL-2.1, the data of ^{56}Fe and natural Fe, ^{54}Fe , ^{57}Fe , ^{58}Fe are evaluated by different authors, so the data of natural element and its isotopes are not consistent with each other. This is one of the main problems in CENDL-2.1. So, after it was completed, using the adjusting program system CABEI, developed at CNDC, the data were adjusted in 1996. As a result the data of natural Fe in CENDL-2.1 (R) become consistent with its isotopes, and at the same time, the consistence for each nuclides are kept.

The data of structural material Fe, Cr, Ni from CENDL-2.1 were plotted and intercompared with ENDF/B-6 (R), JENDL-3.2, JEF-2.2 and BROND-2. It was concluded that the data have been improved much more compared with CENDL-2, especially for Fe and Cr. More attention was paid

to total cross sections and secondary neutron spectra. But the gamma production data need to be improved further. The gamma production cross sections are twice larger than others and experimental data. Comparing with the experimental data, the gamma emission spectra are somewhat soft, there is more low energy gamma (< 5 MeV) for Fe and less high energy gamma (> 5 MeV) for Cr.

To test total cross section, the neutron transmitted spectra through lump of Fe material (8 and 12 in thick respectively) were calculated and compared with broomstick experiment (R. E. Maerker, ORNL-TM-3867) for CENDL-2.1 and other evaluated libraries. The results show that the data for CENDL-2.1 are basically consistent with experimental data and others above neutron energy 3 MeV, but there is still some discrepancies below 3 MeV (the discrepancies also for JENDL-3.2, especially for BROND-2).

CENDL-2.1 has been tested for ten homogeneous, eight heterogeneous thermal^[2] and nine homogeneous fast assemblies^[3], which were recommended by CSEWG of America. 123-group (for thermal) and 175-group (for fast) cross section were generated with code system NJOY91.91 / NSLINK, MILER, the effective multiplication factors and reaction rate ratios were calculated with code system PASC-1.

The calculated K_{eff} are shown in Figs. 1, 2 for homogeneous and heterogeneous thermal assemblies. It can be seen that the K_{eff} are much close to 1.0 for first five homogeneous (Fig.1) and eight heterogeneous (Fig. 2) uranium assemblies, ranging from 0.9944 to 0.9995 and from 0.9965 to 1.0027 respectively, but are considerably overestimated (maximum 2.44%) for last five homogeneous plutonium assemblies (Fig.1). In Fig. 3, the K_{eff} are shown for homogeneous fast assemblies. It can be seen that they are very close to 1.0 (ranging from 0.9994 to 1.0014) for first three ^{235}U assemblies with different spectra. They are overestimated by about 0.4% for two plutonium metal bare sphere assemblies (JEZEBEL and JEZEBEL-Pu), but it becomes better for plutonium assembly with natural uranium reflector (FLATTOP-Pu). They are changed from 0.9946 to 1.0093 for three different ^{233}U assemblies without, with natural U and ^{233}Th reflector.

In conclusion, the agreements of the calculated K_{eff} with experimental ones are quite well for U fast, thermal (homogeneous and heterogeneous) assemblies, but the K_{eff} are overestimated for Pu thermal, fast assemblies. This means that the data of ^{235}U , ^{238}U (and O, H) in CENDL-2.1 are reliable, but the data of Pu need to be improved. The similar conclusion also obtained from analysing the calculated reaction rate ratio data for above assemblies.

To compare, also the calculations have been done with ENDF / B-6 data

for above assemblies and the K_{eff} are shown in Figs. 1-3.

2. The Development of Special Purpose Files

The great effort has been made to develop special purpose files in last year to meet the requirement of nuclear engineering and technology at home and international cooperation.

(1) Fission yield

First of all, the data of existing major fission yield libraries CENDL-FPY, ENDF/B-6, JENDL-3.2, JEF-2.2 and BROND-2 were plotted and intercompared with evaluated or selected experimental data for 41 product nuclides. It was found that the data of all 5 libraries for cumulative fission yield are in or basically in agreement for about one third of the total nuclides and others are discrepant. For independent yield the discrepancies are quite large. Usually, the data from JENDL-3 and CENDL-FY are more close, and the data from ENDF/B-6 and JEF-2 are more close, and the data from BROND-2 are often deviated from the others. Comparing with experimental data, the better agreements are ENDF/B-6 and JENDL-3.2.

The fission yields of some important product nuclides were evaluated for ^{235}U , ^{238}U fission induced by neutron in the energy region up to 20 MeV. For this, some codes for fission yield data evaluation and EXFOR data retrieval were developed. The yield dependence on energy were studied. It was found that the dependencies of FY on incident neutron energy are simply linear for some products, but not for others.

(2) Activation cross section

The activation cross section file of Chinese Evaluated Nuclear Data Library CENDL-ACF was preliminary established. At present, it contains data of more than 150 reaction channels, which were all evaluated in China, most of them were specially evaluated as activation and dosimetry data according to the requirement at home and of international cooperation (RCPs and CRP), and some were collected from the general purpose file of CENDL-2.1 and revised.

Follows were evaluated in last one or two years :

(n, α): D, ^{19}F , ^{31}P , ^{51}V , $^{63,65}\text{Cu}$;
(n,p): ^{14}N , ^{27}Al , ^{51}V , ^{52}Cr , ^{54}Fe , ^{58}Ni ($^{58\text{m}}\text{Co}$), ^{59}Co , ^{63}Cu , ^{64}Zn , ^{137}Ba ;
(n,n'): ^{52}Cr , ^{93}Nb ($^{93\text{m}}\text{Nb}$);
(n,2n): D, ^{19}F , ^{52}Cr , ^{58}Ni , ^{59}Co , ^{63}Cu , ^{87}Rb , ^{89}Y , ^{93}Nb , ^{96}Zr , ^{140}Ce ,

^{151}Eu , ^{180}Hf ($^{179\text{m}}\text{Hf}$), ^{181}Ta ($^{180\text{m}}\text{Ta}$), ^{197}Au , ^{204}Pb ;
 (n,3n): ^{180}Hf , ^{181}Ta , ^{197}Au ;
 (n, α): ^{27}Al , ^{31}P , ^{51}V , ^{54}Fe , ^{59}Co , ^{63}Cu ;
 (n,4n): ^{197}Au ;
 (n,t): ^{54}Fe ;
 (n,n): ^{27}Al .

(3) Intermediate energy nuclear data

The cross sections for neutron monitor reactions up to 100 MeV and for proton monitor reactions up to more than 1 GeV have been evaluated and calculated. They are

$^{54, 56, 57, 58, \text{Nat}}\text{Fe}(n,x)^{51}\text{Cr}$, $^{52, 54, 56}\text{Mn}$,
 $^{63, 65, \text{Nat}}\text{Cu}(n,x)^{56, 57, 58, 60}\text{Co}$,
 $^{197}\text{Au}(n,x)^{194, 195, 196}\text{Au}$,
 $^{59}\text{Co}(n,x)^{56, 57, 58}\text{Co}$, $^{52, 54, 56}\text{Mn}$, ^{59}Fe ,
 $^{169}\text{Tm}(n,x)^{165, 166, 167, 168}\text{Tm}$,
 $^{\text{Zr}}(n,x)^{88, 89}\text{Zr}$, $^{86, 87, 88}\text{Y}$
 and ^{56}Fe , $^{63, 65}\text{Cu}(p,n)$.

Also some cross sections for medical radioisotope production have been evaluated and calculated up to 80 MeV. They are ^{11}B , ^{13}C , ^{77}Se , $\text{W}(p,n)$ and $^{16}\text{O}(p,\alpha)$.

For this, some codes have been developed based on optical model, evaporation and pre-equilibrium theory. They are

CFUPI n, p, α , d, t, ^3He reaction on fissile nuclei, $E < 35$ MeV
 SPEC reaction cross sections and spectra for n, p, α , d, t, ^3He , $E < 70$
 MeV
 DDCS double differential cross sections for n, p, α , d, t, ^3He , $E < 60$ MeV
 CCRMN reaction cross section for n, p, α , d, t, ^3He , $E < 100-200$ MeV
 APMN optical parameter adjusting for n, p, α , d, t, ^3He , $E < 300$ MeV.

(4) Photonuclear reaction data

The complete data of photonuclear reaction up to 30 MeV, including cross section, double differential cross section, gamma production data of all possible reactions, have been evaluated and calculated by using code GUNF for nuclides $^{54, 56-58, \text{Nat}}\text{Fe}$ and $^{63, 65, \text{Nat}}\text{Cu}$.

3. CENDL-3

A five year plan (1996-2000) for nuclear data have been approved by our

authorities and a workable plan in detail have been made by Chinese Nuclear Data Evaluation and Nuclear Theory Working Group. To complete the plan, many groups on different subjects have been organized at CNDC and in Chinese Nuclear Data Network.

According to the plan, CENDL-3 will be completed by 2000, and will contain 200 nuclides. Among them, the data of following nuclides will be newly or reevaluated : fissile nuclides 15, structure materials 18, light nuclides 5, fission products 91. It will contain consistent data between natural elements and their isotopes for structure material, newly evaluated data for fission products, much improved secondary neutron spectra for light nuclides and more γ -production data (files 12-15), double differential cross section (file 6), covariance matrix (files 31-35).

According to the plan, also the special files for fission yield, activation cross section, decay data and intermediate data will be developed.

The main works in 1996 were concentrated on the studying evaluation and calculation methods and developing programs to make the evaluation at more high level. A program system CABEI has been developed for adjusting the consistence between element's and its isotopes' data, SUNF program has been developed for calculating neutron data of fission product nuclides, program ECIS 95 has been transplanted for calculating data of fissile nuclides, the method is being studied to calculate the double cross section of light nuclides, three programs UNF, NDCP, TNG is being intercompared for calculating data of structural material, some researches on (n,α) , $(n,2n)$ systematics is being done. Some experimental data were collected and evaluated. All of these have made a good preparation for the evaluation and calculation for CENDL-3 in the next coming four years. Now the works are going on according to the plan smoothly.

References

1. D. H. Lemmel IAEA-NDS-61, Rev., 3(1995)
2. Liu Guisheng et al., CNDP, 15, 87(1996)
3. Liu Guisheng et al., CNDP, 13, 107(1995)

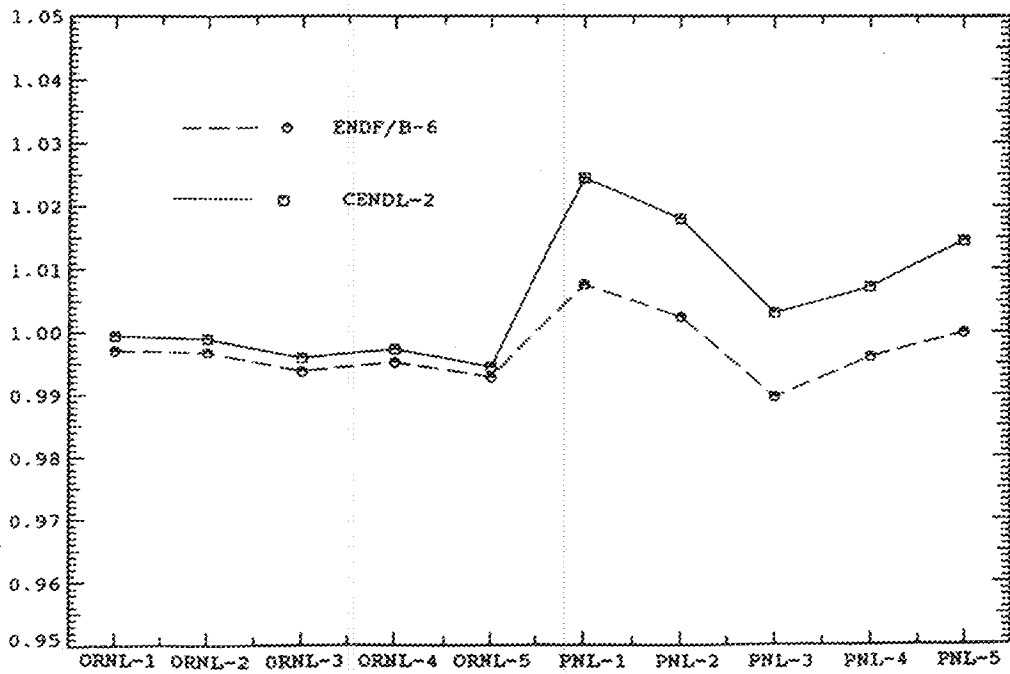


Fig. 1 K_{eff} for thermal homogeneous assemblies

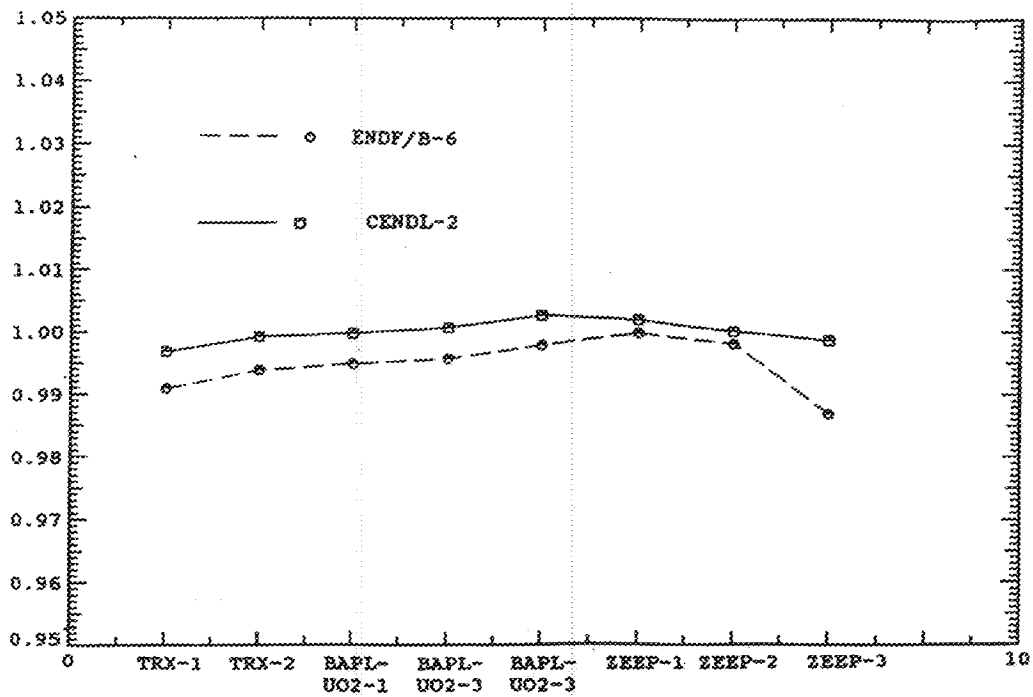


Fig. 2 K_{eff} for thermal heterogeneous assemblies

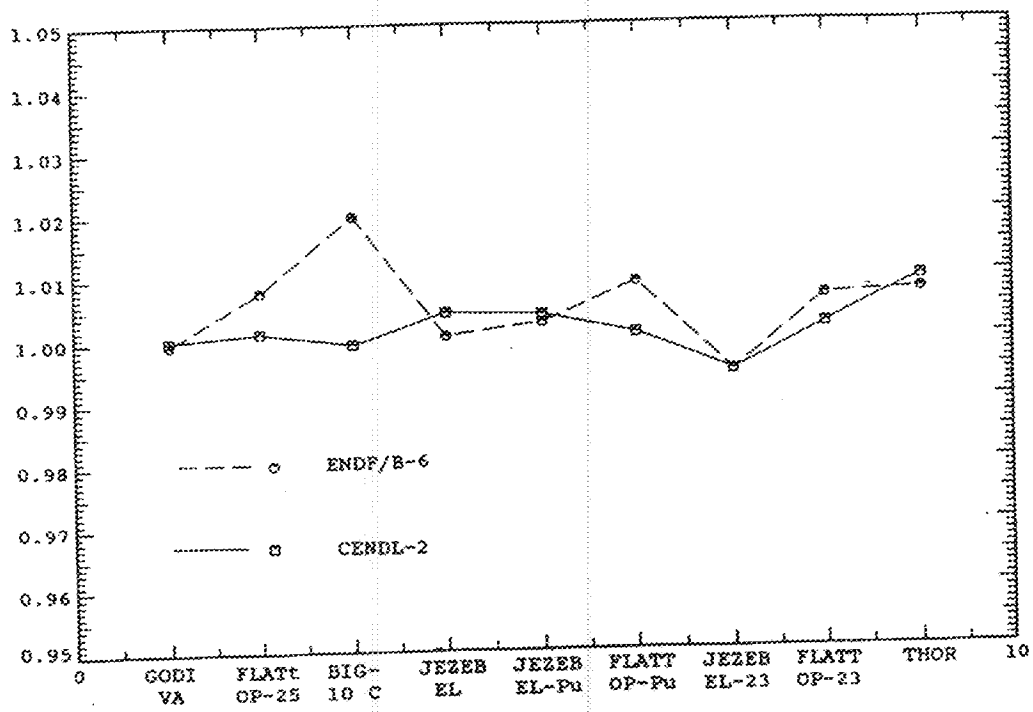


Fig. 3 K_{eff} for homogeneous fast assemblies