

COMPARATIVE ANALYSIS OF HAFNIUM DATA IN EVALUATED NUCLEAR  
DATA LIBRARIES AVAILABLE FROM IAEA NUCLEAR DATA SECTION

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**Abstract:** For research reactor applications of the hafnium data, the evaluated neutron reaction cross-sections in some different libraries available from the IAEA Nuclear Data Section were analyzed comparatively. The libraries selected are INDL-85, JENDL-2(Rev. 1) and UKNDL-81. The NJOY and FEDGROUP-C85 were used to process the ENDF/B formatted libraries and the UKNDL-81, respectively. The hafnium reactivity worth and neutron absorption reaction rates for a control rod model of the KMRR were calculated using the WIMS-KAERI code, and the relative comparisons of the results are given in this paper.

(hafnium isotopes, evaluated data, INDL-85, JENDL-2, UKNDL-81, comparative analysis, reaction rate, reactivity worth)

Introduction

Natural hafnium is currently used as an absorber material for controlling some PWRs or research reactors. Naturally occurring hafnium has six stable isotopes, i.e., Hf-174 and Hf-176 to -180. Most of the isotopes have large thermal and resonance neutron absorption cross-sections, e.g., the 2200 m/sec neutron absorption cross-section and resonance integral of Hf-177 isotope are about 370 and 7200 barns, respectively. Because of their unique neutron absorption characteristics and excellent corrosion resistance to water environments or mechanical properties, hafnium is an attractive material to serve as a neutron absorber for the reactor control. In addition, hafnium absorbs both thermal and epithermal neutrons and its reactivity worth does not appreciably diminish by irradiation. The unique ability of hafnium to absorb neutrons above thermal energies makes it doubly effective as an absorbing material for research reactor control.

Some evaluated nuclear data libraries including the natural hafnium or hafnium isotope

data are recently available from the IAEA Nuclear Data Section.

For research reactor applications, comparative analyses of the neutron reaction cross-sections for the hafnium isotopes in some different data libraries were performed.

However, a more detailed information concerning some evaluated data libraries, i.e., INDL-85 /1/ and UKNDL-81 /2/, than the comment contained in the computer readable data files is not found in a released documentation. Therefore any comment on the evaluated data base is not included in this analysis.

The neutronics calculations using the different library data were carried out for the KMRR (Korea Multi-purpose Research Reactor) control rod model and the results were analyzed comparatively. The libraries selected for this analysis are INDL-85 of the IAEA, JENDL-2(Rev.1) /3/ of Japan and UKNDL-81 of England.

Status of Thermal and Resonance Data

The low energy neutron reaction cross-sections of absorber materials usually exhibit a 1/v

Table 1. Comparison of Reported Thermal and Resonance Integral Data for Isotopes of Hafnium

Isotope	(1) 2200 m/sec Capture Cross-Sections						Unit: barn
	BNL325-3 <sup>8</sup>	BNL325-4 <sup>9</sup>	ENDF/B-V <sup>10</sup>	INDL-85*	JENDL-2 <sup>3</sup>	UKNDL-81 <sup>11</sup>	
Hf-174	390. (0.90)**	561. (1.30)	391. (0.90)	-	390. (0.90)	-	
Hf-176	38. (1.40)	23.5(0.86)	21.8(0.80)	28. (1.03)	38. (1.40)	14.1(0.52)	
Hf-177	365. (0.99)	373. (1.01)	376. (1.02)	363. (0.99)	352. (0.96)	376. (1.02)	
Hf-178	86. (1.03)	84. (1.01)	84.6(1.01)	82. (0.98)	86. (1.03)	78.4(0.94)	
Hf-179	45. (1.06)	41. (0.97)	40.4(0.95)	44. (1.04)	45. (1.06)	39.1(0.92)	
Hf-180	12.6(0.91)	13.0(0.94)	13. (0.94)	19. (1.37)	12.6(0.91)	13.1(0.94)	

## (2) Resonance Capture Integral Data

Isotope	BNL325-3	BNL325-4	ENDF/B-V	INDL-85	JENDL-2	UKNDL-81
Hf-174	465. (1.01)	436. (0.95)	446. (0.97)	-	492. (1.07)	-
Hf-176	700. (1.19)	880. (1.49)	337. (0.57)	640. (1.08)	360. (0.61)	625. (1.06)
Hf-177	7260. (1.01)	7173. (1.00)	7220. (1.01)	7180. (1.00)	6950. (0.97)	7240. (1.01)
Hf-178	1950. (1.02)	1950. (1.02)	1747. (0.91)	1950. (1.02)	1920. (1.00)	1962. (1.03)
Hf-179	600. (1.07)	630. (1.12)	451. (0.80)	630. (1.12)	517. (0.92)	544. (0.97)
Hf-180	43. (1.17)	35. (0.95)	29. (0.79)	43. (1.17)	34.6(0.94)	36.2(0.98)

\* Data from the text given at the information of each isotope in the library.

\*\* Values in the parenthesis are the ratio to the average value.

energy dependence and the cross-sections in the resonance energy ranges are often represented as the sum of a resonance contribution. Because of its  $1/v$  behavior in thermal energy range and complicated shape of the resonance, the 2200 m/sec neutron absorption data and values of the resonance integral are often used as a starting point for evaluating the cross-sections in each energy region.

As a prior comparison of the evaluated hafnium data, the thermal capture cross-sections and resonance integral of the hafnium isotopes, extracted from the given references, are compared in Table 1 together with the ratios of those to the average value. As can be seen in the table, there exist large inconsistencies between the evaluations.

#### 69-group Data Generation

Among the libraries considered, INDL-85 does not contain the Hf-174 isotope data. However, the percent contribution of the Hf-174 to natural hafnium absorption is less than 1%. Therefore, the Hf-174 was excluded from this analysis.

The NJOY system/4/ was used to process the ENDF/B formatted library, i.e., INDL-85 and JENDL-2, and FEDGROUP-C85 system/5/ was employed for the UKNDL-81. Using the systems and libraries 69-group cross-section data sets for the WIMS-KAERI code/6/ were generated.

Most of neutronics design codes have their built-in multi-group library which usually contains the only absorption data for the absorber materials such as fission-products or burnable isotopes. Therefore, two kinds of 69-group data sets which contain all kinds of reaction cross-sections and the only absorption cross-section data with no scattering assumed, respectively, are generated.

#### Calculation Model

As a reference model for calculating the hafnium reactivity worth, the KMRR control rod assembly was considered. The concise specification of the fuel element is given in Table 2.

The material of control rods of the KMRR is natural hafnium in tube form. Since the hafnium has good compatibility to water, it is in the bare form. The 18-element fuel assemblies that reside inside the circular flow tube automatically increase total fuel loading of the core when the absorber tubes are withdrawn during operations. In this model, additional 3 arrays of fuel pins and a water zone were taken into account as environment. The model is shown in Fig.1.

Table 2. Concise Specification for KMRR Fuel Element

Fuel Meat(U3Si-Al)	: U ; 58.6%
	Si; 2.4%
	Al; 39.0%
Enrichment	: 20% U-235
Density(g/cm <sup>3</sup> )	: 5.29
Diameter(mm)	: 6.35
Length(mm)	: 700.0
Cladding	: Al
Thickness(mm)	: 0.76
No. of Fin	: 8
Height(mm)	: 1.02
Width(mm)	: 0.76

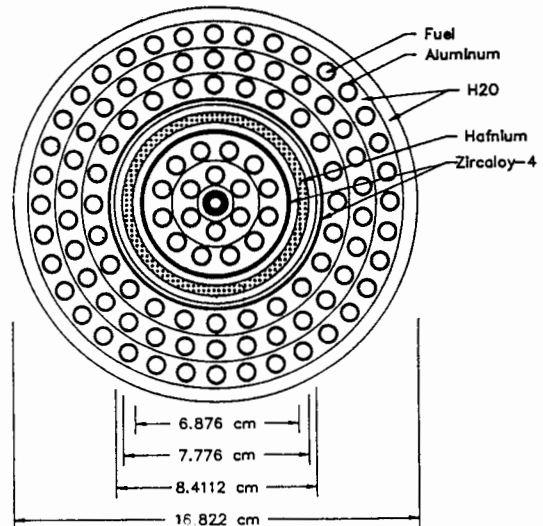


Fig.1 Calculation Model

#### Results and Discussion

The WIMS-KAERI code, which is a revised version of the WIMS/D4 code/7/, and its built-in 69-group nuclear data library are used for the neutronics calculations of the model in Fig.1. The transport calculations were performed based on the collision probability method using the processed different data sets. In the calculations, the zero current condition was applied at the outer boundary of the model.

#### 69-group Absorption Cross-section

The processed absorption cross-sections for the hafnium isotopes are compared in Figure 2 to 6. As can be seen in the figures, all isotopes have large resonance peak values, e.g., the maximum peak of Hf-177 is about 25000 barns at  $\sim 1.1$  eV. Cross-sections for Hf-176 and Hf-180 show large inconsistencies between the three libraries. JENDL-2 values for Hf-176, -177 and -179 show a big difference from the other two library data in the fast energy region.

As can be deduced from Table 1 as well, the Hf-176 and -180 data in the  $1/v$  dependent energy region show significant inconsistencies between the libraries. The agreement for the

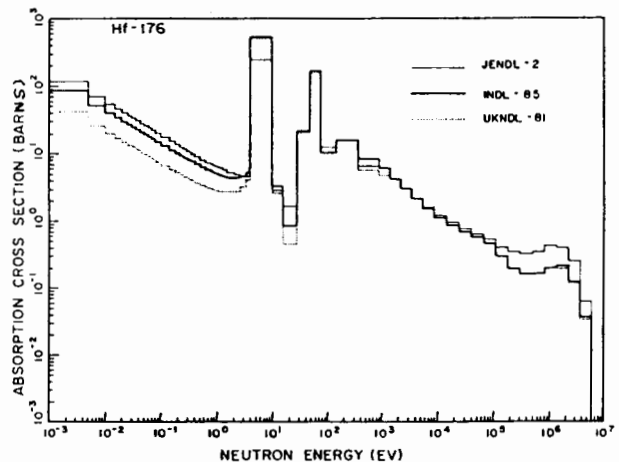


Fig.2 69-group Cross-Sections of Hf-176

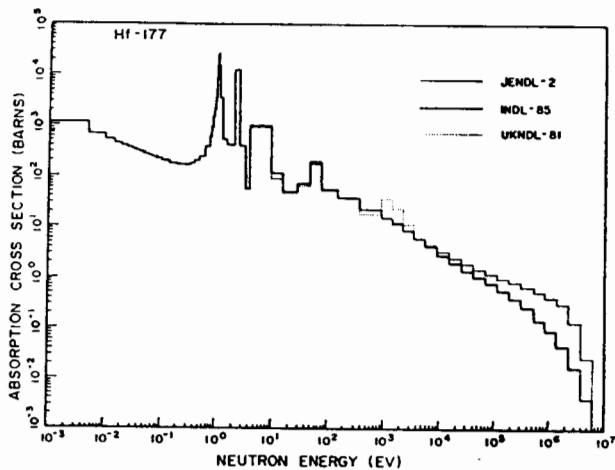


Fig.3 69-group Cross-Sections of Hf-177

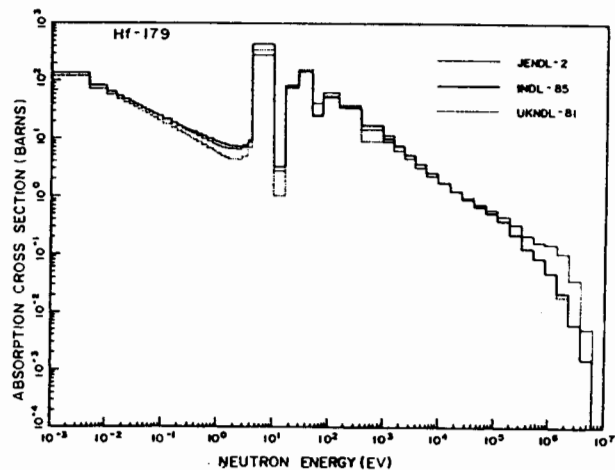


Fig.5 69-group Cross-Sections of Hf-179

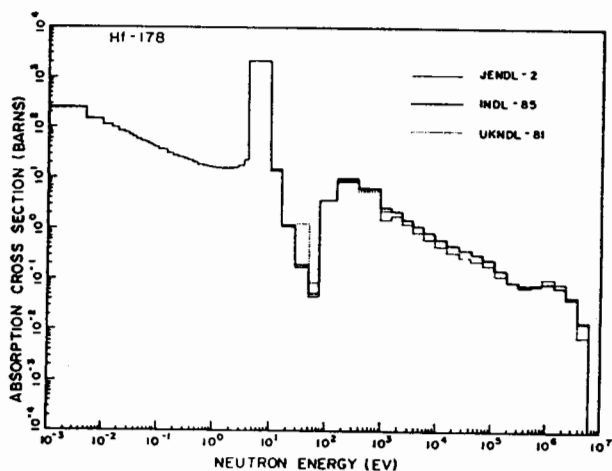


Fig.4 69-group Cross-Sections of Hf-178

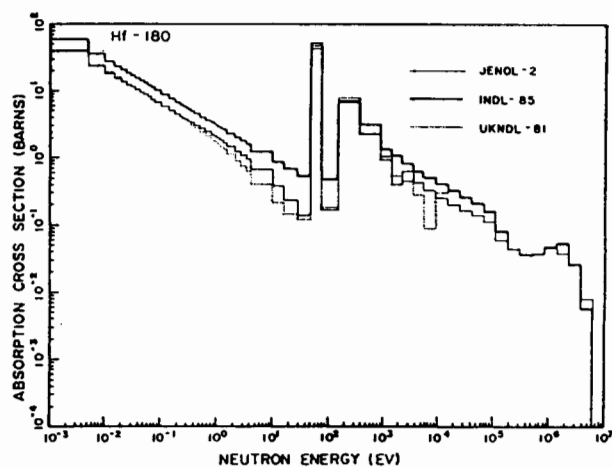


Fig.6 69-group Cross-Sections of Hf-180

Hf-177 data in the thermal and resonance energy range is good comparatively.

The scattering cross-sections for the hafnium isotopes show very large inconsistency each other but a negligible effect on the reactivity worth.

#### Absorption Reaction Rate

As a quantitative comparison of the absorption cross-sections, the energy dependent neutron absorption reaction rates for all hafnium isotopes were calculated, and the results are given in Table 3. The listed values are the percent contributions of each isotope to the natural hafnium absorption. And the total absorption rate in the natural hafnium is normalized to 100%. The fast, resonance and thermal energy in the table have the boundaries between 10 MeV - 9.118 keV, 9.118 keV - 4.0 eV and 4.0 eV - 0.0 eV, respectively. Hf-177 absorption in the thermal and resonance energy range contributes more than 60% to the total absorption of natural hafnium. The contribution of three isotopes of Hf-177, -178 and -179 is more than 90% of the effective absorption in natural hafnium. This is due to their large absorption cross-sections and relatively larger abundance. While the absorption of each isotope in the fast energy region contribute only few percent, i.e., less than 1% to the total reaction rate. The ~40% contribution of Hf-177 absorption comes from the large resonances between 1 eV - 3 eV.

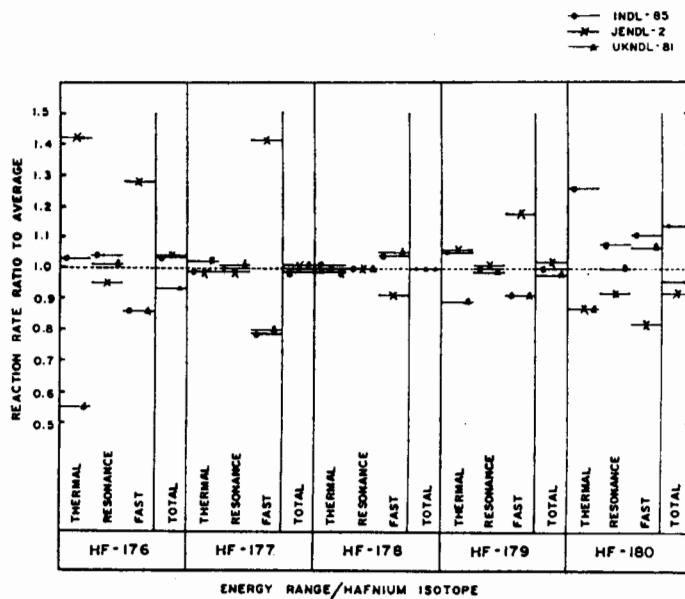


Fig.7 Comparison of Energy Dependent Reaction Rate Ratios to Average Value

Fig.7 shows a relative comparison of the reaction rates for the three data sets. And summarized are the followings for the degree of agreement between data bases:

Table 3. Contribution of Energy Dependent Absorption Reaction Rates(%) of Each Isotope to Natural Hafnium

Library	Energy Range	Isotope					Natural Hafnium
		Hf-176	Hf-177	Hf-178	Hf-179	Hf-180	
INDL-85	Fast	0.1	0.8	0.4	0.3	0.3	1.9
	Resonance	2.3	20.5	9.6	10.8	3.8	47.0
	Thermal	0.5	39.2	7.3	2.0	2.1	51.1
Total		2.9	60.5	17.3	13.1	6.2	100.0

- . in the thermal energy region,
  - Hf-176 : bad
  - Hf-177, -178 : good
  - Hf-179 : low UKNDL-81
  - Hf-180 : too high INDL-85
- . in the resonance energy region,
  - Hf-176 to -179 : good
  - Hf-180 : bad
- . in the fast energy region,
  - Hf-176, -177, -179 : too high JENDL-2
  - Hf-178 : low JENDL-2
  - Hf-180 : too low JENDL-2

Though JENDL-2 data appear to be somewhat too high or low in the fast energy region, it is not important in the viewpoint of total reactivity worth for the natural hafnium because of their low contribution to the total worth.

Fortunately, the agreement of the thermal and resonance absorption data for the Hf-177, -178 and -179, which are principal contributors to the total absorption of the natural hafnium, is comparatively good between the libraries considered.

Reactivity Worth

The reactivity worth calculations were carried out using the hafnium data in the three different data sets. The reactivity worth of the absorber was calculated by

$$\text{Worth} = (1/K_{in} - 1/K_{out}) \times 1000 \text{ (mk)}$$

where  $K_{in}$  is the K-infinity value when the absorber material is inserted and  $K_{out}$  is the K-infinity value when the absorber material is withdrawn.

The results are given in Table 4. In the table, the calculated values using the data sets with and without scattering data are included together. The reactivity worth calculated by using the INDL-85 data is about 0.6% larger than that of the other two libraries, and the effect of scattering data is around 1%.

While in order to survey a maximum worth difference which can be deduced from the three different data sets, two kinds of pseudo sets

composed of the maximum and the minimum absorption cross-section values among the three data sets are generated. And the worth calculations using the pseudo set data were performed. The calculated worth difference between the two pseudo sets is given in Table 5. The maximum difference which can be deduced from the above-mentioned pseudo set data is about 5%.

Table 5. Worth Difference Available from the Three Libraries

Pseudo Data Set	Worth (mk)	Ratio (Max/Min)
Max. Absorp.	329.85	1.05
Min. Absorp.	314.03	

Conclusion

- . The absorption cross-sections of both Hf-176 and Hf-180 isotopes show large inconsistencies between the evaluated data libraries.
- . In the fast energy region, relatively significant differences are observed between the JENDL-2 and the other two libraries but this gives no severe impact on the total worth of the natural hafnium.
- . More than 60% of the neutron absorption in natural hafnium is due to the contribution of the Hf-177 isotope.
- . The contribution of three isotopes of Hf-177, -178 and -179 is more than 90% of the effective absorption in natural hafnium.
- . The reactivity worth of the natural hafnium obtained from the three different libraries are consistent to within about 0.6%, and an available maximum discrepancy between the data sources is about 5%.
- . The reactivity worth effect of scattering cross-sections in natural hafnium is within a few percent.

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Table 4. Calculated Reactivity Worth of Natural Hafnium

Library	With / Without Scattering Set		Ratio
	With	Without	
	Unit: mk		
INDL-85	325.65	322.99	1.008
JENDL-2	323.78	321.12	1.008
UKNDL-81	323.84	320.42	1.011