Evaluation of Significance of Zr Bound in ZrH_x for its Possible Inclusion in the WIMSD-5 Cross Section Library

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Abstract

The principal objective of this study was to evaluate the significance of a separate data for Zirconium bound in Zirconium hydride rather than as a free atom and its possible inclusion in the WIMSD library. A TRIGA research reactor benchmark input specified for WIMSD-5 was prepared. The calculations have been performed by the WIMSD-5B code and the ANL version of WIMSD code. In the ANL version, two sets of data for Hydrogen were available: for Hydrogen bound in water and Hydrogen bound in Zirconium hydride. For Zirconium, the available data were for Zirconium natural and Zirconium bound in Zirconium hydride prepared without taking into account the P_1 correction. A separate data for Zirconium bound for Zirconium hydride with P_1 correction was prepared for the WIMSD-5B code at INST, AERE, Savar. The cross section data for all the elements of the benchmark input have been processed by NJOY94.10+ based on ENDF/B-VI library and incorporated in the 69-group WIMS library. All the calculations have been carried out applying 69 energy groups in the main transport routine with subsequent condensation to 7 group. Four cases namely (i) diffusion, (ii) B_1 with P_1 thermal scattering matrices for H and O in water only, (iii) as above but with a P_1 matrix also for H bound in ZrHx, (iv) as above but with a P_1 matrix also for Zr bound in ZrHx were studied. It is seen that the differences in cross sections are negligible although the overall effect in K-eff is up to 700 pcm in the case of ANL, and in our case, the effect is even stronger. The possible cause of this inconsistency could be the absence of P_1 matrices for all the principal materials for the benchmark input in the WIMSD library. The author of the WIMS recommends the usage of P_1 matrices only if they are available for all principal isotopes of a material. No material is treated separately on the level of leakage calculations and the contribution from the first order is weighted over spectra in materials, their volume and number densities.

Introduction

The principal objective of this study was to evaluate the significance of a separate data for zirconium bound in zirconium hydride rather than as a free atom and its possible inclusion in the WIMSD library. The influence of leakage and, in particular, P1 matrices on k-eff depends on the magnitude of the buckling, consequently might have a significant effect for a small reactor like TRIGA, so is the essence of performing this calculation. A Benchmark input specified for WIMSD-5 has been prepared. The calculations have been performed by the WIMSD-5B code developed at ANL[1]. Only two sets of data for hydrogen were available: for hydrogen bound in water and hydrogen bound in zirconium hydride. For zirconium, the available data were for zirconium natural and zirconium bound in zirconium hydride prepared without taking into account the P_1 correction. A separate data for zirconium bound in zirconium hydride with P_1 correction was prepared. The cross section data for all the elements of the benchmark input have been processed by NJOY [2] based on ENDF/B-VI library and incorporated in the 69-group WIMS library. All the calculations have been carried out applying 69 energy groups in the main transport routine with subsequent condensation to 7 group.

Significance of separate data for Zr bound in ZrH_x

The problem can be divided into two questions: (1) what is the effect of introduction of Zr bound in ZrH_x as a separate isotope with its own ID and the whole set of data?
(2) Is it necessary to introduce a P_1 scattering matrix for that new isotope?

Evaluation of the first effect is comparatively easy. It can be carried out by comparison of the computational results for a typical reactor with ZrH_x in its fuel, based on the free atom approach and those obtained with Zr bound in ZrH_x. Such a comparison has been done using the WIMS-ANL code and its standard library prepared on the basis of ENDFB-VI.

The second question is more complicated as it is connected with the specific algorithm applied in WIMSD in all its versions for B_1 calculations. This algorithm is described in detail below to give a theoretical basis for answering the second question.

Application of P1 matrices

The transport calculations in the WIMSD code are performed in consecutive steps. First, a detailed solution of the transport equation is carried out for the input case, treated as an infinite lattice of specified cells (macro-cells). Second, the code solves the transport equation once more using effective cross sections for a uniform infinite plate with given radial and axial bucklings. The first comparison shows the differences between calculations carried out on the basis of library data prepared separately for zirconium bound in the zirconium hydride (ID=2091) and those prepared for natural zirconium (ID=91) without taking into account the P_1 correction. The transport equation can be solved in the diffusion approximation written as:

$$\left(\sum^{g} - \sum_{s0}^{gg} + D_r^g.B_r^g + D_z^g.B_z^g \right).\Phi^g = \sum_{g' \neq g} \sum_{s0}^{g'g} .\Phi^{g'} + S_f^g \qquad (1)$$

Where:

Σ^g-total cross section in group g,

$\sum \frac{g'g}{so}$ –Scattering cross section, from group g' to g,

$D\frac{g}{x}$ –Diffusion coefficient in the direction x for group g,

$\mathrm{B}\frac{g}{x}$ – buckling in the direction x for group g,

ϕ^g – Neutron flux in group g,

$S\frac{g}{f}$ – Fission source in group g.

P1 matrices for four light elements (H-1, H-2, O and C) are included in the WIMS library. The matrices are used only in the third part of WIMS calculations, so called, 'leakage correction'. The code solves transport equation for the whole system specified in input data before it performs any leakage correction. Thus the neutron flux values and macroscopic cross section are known for all regions in the infinite medium approximation. A leakage correction is then introduced through the application of input buckling given in input or bucklings calculated in the code and corresponding to the effective multiplication factor equal to unity. This is realised by flux volume weighting of macroscopic cross sections for all regions. Thus an artificial uniform medium is created in the form of an infinite slab and for that slab system once more the transport equation is solved but this time with a buckling correction. The transport equation for the uniform plate can be solved in the B1 approximationhere the notation of Eq. (1) has been kept, $B^2 = B\frac{2}{r} + B\frac{2}{z}$, and the neutron current is calculated as:

$$J^g = \frac{\sum\sum_{s1}^{g'\neq g} \frac{g'g}{s1} . J^{g'} + \frac{(B)^2}{|B^g|} . \phi^g}{3a^g \sum^g - \sum \frac{gg}{s1}} \qquad (3)$$

The quantities a are defined by the following formulas:

$$a^g = \left(\frac{B}{\sum^g}\right)^2 . \frac{arctg\left(\frac{B}{\sum^g}\right)}{3\left(\frac{B}{\sum^g} - arctg\left(\frac{B}{\sum^g}\right)\right)}; \; for B^2 > 0, \qquad (4a)$$

$$a^g = \left(\frac{B}{\sum^g}\right)^2 . \frac{in\left(\frac{\sum^g + |B|}{\sum^g - |b|}\right)}{\left(\frac{\sum^g + |B|}{\sum^g - |b|}\right) - \left(\frac{2|B|}{\sum^g}\right)}; \text{ For } B^2 > 0. \qquad (4b)$$

It should be noted that B=0 is not allowed in this approximation.

It should be kept in mind that as already stated, all material constants in both equations are properly weighted averages over respective regions of the whole system (cell or macro cell). In the second equation, beside the macroscopic cross-sections are calculated only now and only for the thermal energy diapason. In the present versions of the WIMSD-5 library there are only for 4 isotopes: hydrogen, deuterium, oxygen and carbon. Their application in calculations is activated by specification of the DNB cards in the third section of WIMS input. Their densities for each material are taken from the DNB cards and not from MATERIAL cards.

It should be kept in mind that the effect of P1 approach is meaningful only in the case of larger buckling values. It has no influence on the infinite lattice results and the leakage correction, expressed through Eqs. (1,2). The calculation of the effective spectrum and effective multiplication factor is a very rough one for a majority of reactors.

Numerical Results

The comparison is, therefore, done using the transport diffusion approximation. The difference in multiplication factors is shown on Table 1. For comparison, a case with hydrogen treated as bound in water (ID=2001) and not in zirconium hydride (ID=2191) has also been calculated

Table 1

Multiplication factors with different data for Zr and ZrH_x.

Library ID applied	Zr:91,H: 2001	Zr:91,H:2191	Zr:2091,H:2191
k-inf	1.400835	1.394566	1.393325
k-eff	1.087118	1.080440	1.079449

The differences in macroscopic cross sections can be observed Table 2,3 and 4

Table 2a
Broad group cross sections with ID (Zr)-91,ID (H)-2001 in ZrH_x

Broad Grp	Transport	Total	Capture	Fission	ν
1	2.14685E-01	3.56968E-01	4.76302E-04	9.34045E-04	2.72291E+00
2	5.67011E-01	1.05267E+00	1.84368E-03	8.45263E-04	2.43774E+00
3	6.57276E-01	1.41642E+00	2.05585E-02	8.88930E-03	2.43380E+00
4	8.12719E-01	1.49297E+00	1.63073E-02	2.11660E-02	2.43380E+00
5	1.15829E+00	1.84333E-00	4.17381E-02	4.65435E-02	2.43380E+00
6	1.81717E+00	2.49116E+00	3.16287E-02	6.54957E-02	2.43380E+00
7	3.02414E+00	3.71359E+00	5.17901E-02	9.90251E-02	2.43380E+00

Table 2b
Macroscopic scattering matrix with ID (Zr)=91, ID (H)=2001 in ZrH_x

To Grp	From Grp 1	From Grp 2	From Grp 3	From Grp 4	From Grp 5	From Grp 6	From Grp 7
1	2.59159E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	9.61447E-02	9.20826E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	2.53671E-04	1.29056E-01	1.29056E+00	2.99052E-03	1.88543E-12	0.00000E+00	0.00000E+00
4	0.00000E-00	4.48799E-05	6.84758E-02	6.35611E-01	2.81188E-03	2.44568E-10	3.53254E-11
5	0.00000E-00	4.36807E-05	6.32057E-02	6.87894E-01	1.18345E+00	6.61036E-02	8.77267E-03
6	0.00000E-00	8.08790E-06	9.95167E-03	9.95167E-02	4.47863E-01	1.76613E+00	4.26031E-01
7	0.00000E-00	4.09907E-06	4.41136E-03	3.53292E-02	1.15517E-01	5.61800E-01	3.12797E+00

Table 3a
Broad group cross sections with ID (Zr)=91, ID (H)=2191 in ZrHx

Broad grp	Transport	Total	Capture	Fission	ν
1	2.14681E-01	3.56967E-01	1.76306E-01	9.34029E-04	2.72291E+00
2	5.67011E-01	1.05267E+00	1.84369E-03	8.45266E-04	2.43774E+00
3	6.54964E-01	1.41615E+00	2.05852E-02	8.87959E-03	2.43380E+00
4	7.79528E-01	1.47625E+00	1.61477E-02	2.09255E-02	2.43380E+00
5	1.08664E-+00	1.76651E+00	4.67594E-02	4.80971E-02	2.43380E+00
6	1.68158E+00	2.37179E+00	3.33924E-02	7.22649E-02	2.43380E+00
7	3.05185E+00	3.73318E+00	4.77050E-02	8.37288E-02	2.43380E+00

Table 3b
Macroscopic scattering matrix with ID (Zr)=2091, ID(H)=2191 in ZrHx

To Grp	From Grp 1	From Grp 2	From Grp 3	From Grp 4	From Grp 5	From Grp 6	From Grp 7
1	2.59158E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	9.61446E-02	9.20826E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	2.53671E-04	1.29056E-01	1.24025E+00	2.37427-E03	3.52530E-11	0.00000E+00	0.00000E+00
4	0.00000E+00	4.48799E-05	6.79254E-02	6.09647E-01	2.03511E-03	2.47497E-09	1.16030E-10
5	0.00000E+00	4.36807E-05	6.34927E-02	6.87686E-01	1.14770E+00	4.80414E-02	1.07285E-02
6	0.00000E+00	8.08790E-06	1.03820E-02	1.04298E-01	3.81925E-01	1.82878E+00	3.51092E-01
7	0.00000E+00	4.09906E-06	4.63983E-03	3.51725E-02	1.39999E-02	3.89312E-01	3.23992E+00

Table 4a
Board group cross sections with ID(Zr)=2091,ID (H)=2191 in ZrH_x

Broad grp	Transport	Total	Capture	Fission	ν
1	2.14684E-01	3.56967E-01	4.76305E-04	9.34030E-04	2.72291E+00
2	5.67011E-01	1.05267E+00	1.84399E-03	8.45253E-04	2.43774E+00
3	6.54536E-01	1.41575 E+00	2.07270E-02	8.88149E-03	2.43380 E+00
4	7.76895E-01	1.47326 E+00	1.61458 E-02	2.09220E-02	2.43380 E+00
5	1.08406E+00	1.76369 E+00	4.67496 E-02	4.81209 E-02	2.43380 E+00
6	1.67920E+00	2.36922 E+00	3.33885 E-02	7.22503 E-02	2.43380 E+00
7	3.05072E+00	3.73194 E+00	4.76856 E-02	8.36562 E-02	2.43380 E+00

Table 4b
Macroscopic scattering matrix with ID (ZR)=2091,ID (H)=2191 in ZrH_x

To grp	From Grp 1	From Grp2	From Grp3	From Grp4	From Grp5	From Grp6	From Grp7
1	2.59158E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	9.61446E-02	9.20826E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	2.53671E-04	1.29056E-01	1.23978E+00	2.30089E-03	3.52186E-11	0.00000E+00	0.00000E+00
4	0.00000E+00	2.48800E-05	6.78838E-02	6.07055E-01	1.97060E-03	2.47870E-09	1.15843E-10
5	0.00000E+00	4.36807E-05	6.34668E-02	6.87369E-01	1.14641E+00	4.75525E-02	1.07271E-02
6	0.00000E+00	8.08791E-06	1.03777E-02	1.04299E-01	3.80434E-01	1.82882E+00	3.49182E-01
7	0.00000E+00	4.09907E-06	4.63792E-03	3.51736E-02	1.40005E-01	3.87203E-01	3.24069E+00

It is seen that the differences in cross sections are negligible although the overall effect in k-eff is up to 700 pcm.

Test for the effect of P_1 scatting matrices in WIMS-ANL.

The test included calculation if the TRIGA typical fuel under the B1 option with correct cross section for zirconium and hydrogen in zirconium hydride, ie. with ID (Zr)=2091 and ID(H)=2191,in 4 approximations:
(i) diffusion,
(ii) B_1 with P_1 thermal scattering matrices for H and O in water only,
(iii) as above but with a P_1 matrix also for H bound in ZrHx,
(iv) as above but with a P_1 matrix also for Zr bound in ZrHx.
The infinite and effective multiplication factors are shown in Table 5.

Table 5
Infinite and effective multiplication factors in various approximations of leakage calculations.

Case	(i)	(ii)	(iii)	(iv)
K-inf	1.393325	1.393204	1.393057	1.393056
k-eff	1.079449	1.080925	1.090408	1.068336
Φ_E/Φ_{th} in cell	3.42	3.44	3.46	3.46

It is seen that the effect on k-eff from (iii) to (iv) is even stronger than that from (ii) to (iii) but the P1 approximation in hydrogen increases the effective multiplication factor while for zirconium the trend goes in an opposite direction.

The flux spectrum obtained with P_1 matrices used in water and
(i) Without P_1 in ZrH_x,
(ii) P_1 matrix only for H bound in ZrH_x.
(iii) P_1 matrix for both H and Zr in ZrH_x

Table 6
7-group average cell flux values

Lower energy bound[eV]	P1 in H2O	P1 in H_2	P1 in Zr &H
5.0000E+05	3.2019E-01	3.2178E-01	3.2211E-01
1.4251E+03	2.5736E-01	2.5718 E-01	2.5717 E-01
1.1230Ei00	1.8302E-01	1.8254 E-01	1.8242 E-01
6.2500E-01	1.4331E-02	1.4289 E-02	1.4273 E-02
1.4000E-01	4.3202E-02	4.3018 E-02	4.2997 E-02
5.0000E-02	9.3432E-02	9.3048 E-02	9.2980 E-02
1.0000E-05	8.8171E-02	8.8148E-02	8.8016E-02

Conclusion

The results obtained for k-effective and k-infinity is opposite. Also, the values for k-effective given in table 3 increase from (i) to (ii) and (iii) and decrease for (iv). The possible cause of this inconsistency could be the absence of P1 matrices for all the principal materials in the WIMSD library. In description of the DNB[4] card, the author of the WIMS recommends the usage of P1 matrices only if they are available for all principal isotopes of a material. No material is treated separately on the level of leakage calculations and the contribution from the first order is weighted over spectra in materials, their volume and number densities. Therefore, the influence of P1 matrices should be considered only in the sense of its contribution to the whole first order scattering in the calculated cell.

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