Use the results of measurements on KBR facility for testing of neutron data of main structural materials for fast reactors

Vladimir Koscheev¹, Gennady Manturov¹, Vladimir Pronyaev², Evgeny Rozhikhin¹, Mikhail Semenov¹, and Anatoly Tsibulya¹

¹ JSC “SSC RF-IPPE”, 249033 Obninsk, Kaluga region, Russia
² PI “Atomstandart”, 119017 Moscow, Russia

Abstract. Several \(k_\infty\) experiments were performed on the KBR critical facility at the Institute of Physics and Power Engineering (IPPE), Obninsk, Russia during the 1970s and 80s for study of neutron absorption properties of Cr, Mn, Fe, Ni, Zr, and Mo. Calculations of these benchmarks with almost any modern evaluated nuclear data libraries demonstrate bad agreement with the experiment. Neutron capture cross sections of the odd isotopes of Cr, Mn, Fe, and Ni in the ROSFOND-2010 library have been reevaluated and another evaluation of the Zr nuclear data has been adopted. Use of the modified nuclear data for Cr, Mn, Fe, Ni, and Zr leads to significant improvement of the C/E ratio for the KBR assemblies. Also a significant improvement in agreement between calculated and evaluated values for benchmarks with Fe reflectors was observed. C/E results obtained with the modified ROSFOND library for complex benchmark models that are highly sensitive to the cross sections of structural materials are no worse than results obtained with other major evaluated data libraries. Possible improvement in results by decreasing the capture cross section for Zr and Mo at the energies above 1 keV is indicated.

1. Introduction

Several \(k_\infty\) experiments were performed on the KBR critical facility at the Institute of Physics and Power Engineering (IPPE), Obninsk, Russia during the 1970s and 80s to study neutron absorption properties of the basic structural materials of fast reactors. The experiments were evaluated in 2002 according to the ICSBEP rules (HEUCOMP-INTER-005 series [1]). The experiments were performed at special conditions simulating an “infinite” multiplication media with \(k_\infty \sim 1\) fueled with highly enriched uranium. Five critical KBR assemblies were studied where the central test zone contained different structural materials: components of stainless steel (SS) – Cr, Mn, Fe, Ni; as well as Zr and Mo. Sizes of these zones were chosen in order to eliminate the influence of the surrounding driver region to the neutron-physical characteristics in the core center. Influence of neutron leakage in this case could be neglected, so the multiplication factor is determined mostly by the neutron capture process in the studied materials.

There have been multiple attempts to reproduce the results of these experiments using different neutron data libraries. However, calculated \(k_\infty\) values using almost any set of data are inconsistent with the experimental results within the limits of the estimated uncertainty (in particular, this is noted in papers presented at recent international conferences [2,3]). Meanwhile, these experiments are highly sensitive to the neutron capture of structural materials in the energy range of 1–100 keV. Table 1 shows the balance relation for neutron capture in the “infinite” cell of the central zone of each assembly of this series (taken from [1]). It may be mentioned that the neutron capture for KBR-7 (HCI-005-01) is determined mainly by Ni; for KBR-15 (HCI-005-04) – by Cr; for KBR-16 (HCI-005-05) – by Zr; for KBR-9 (HCI-005-02) – by Fe, and for KBR-10 (HCI-005-03) – by Fe and Mo.

The results of testing of the modified neutron cross sections for stable isotopes of basic structural materials from the ROSFOND-2010 library [4] using the HCI-005 series benchmarks are presented in this paper. In addition, the results of \(k_{\text{eff}}\) calculations for several benchmark experiments from the ICSBEP Handbook having a significant sensitivity to the neutron cross sections of structural materials are also given.

2. Modification of neutron cross sections

The following approach was used for modification of the neutron cross sections files:

– The neutron data files from the ROSFOND-2010 library (hereafter RF10) were taken as a basis;
– Microscopic cross-section measurements, including the most recent experiments, were analyzed;
– The observed increasing trend in capture for the isotopes of Cr, Mn, and Fe, and decreasing trend in capture for the isotopes of Ni and Zr in the energy range from 1 to 100 keV were taken into account.

The parameters of the first resonances for the odd isotopes of Cr, Mn, Fe, and Ni were modified, which determine the capture of the natural mixture of isotopes at the
energies from 1 to 20 keV. To improve the description of the assemblies with Fe reflectors, the anisotropy in the elastic scattering cross sections for Fe-56 was also modified based on Hetrick, Fu, and Larson evaluation [5]. Revision of the Cr-53 evaluation led to significant changes in the parameters of the first four positive resonances with substantial increase in capture. This is confirmed by recent measurements of Guber et al. [6].

Evaluation by Ichihara et al. [7], adopted in the JENDL-4.0 library, was used as a basis for neutron cross section data for Zr isotopes.

A comparison of the radiative capture resonance integral (Rc) in the energy range 0.5 eV–100 keV for the modified files (RF10+) with the same data from the original RF10 library and with Mughabghab’s evaluation (Atlas-2006) [8] is shown at Table 2.

We may conclude from the comparison data of Table 2, that:

– capture for natural Cr is increased mainly due to the increase of the Cr-53 capture, and the Rc value for the modified data is closer to the Atlas-2006 recommended value;
– capture for Mn is increased and the Rc value for the modified data is also consistent with the Atlas-2006 recommended value;
– capture for natural Fe is slightly increased (there is no evaluation of the Rc in Atlas-2006);
– capture for natural Ni is slightly decreased (there is no evaluation of the Rc in Atlas-2006);
– capture for natural Zr is decreased, and the Rc value for the modified data is consistent with the Atlas-2006 recommended value within the given uncertainty.

### Table 1. Contribution of capture by KBR structural materials to the total neutron balance, %.

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>KBR-15/ Cr</th>
<th>KBR-9/ SS</th>
<th>KBR-10/ Mo</th>
<th>KBR-7/ Ni</th>
<th>KBR-16/ Zr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr</td>
<td>32.3</td>
<td>7.2</td>
<td>3.7</td>
<td>0.5</td>
<td>1.2</td>
</tr>
<tr>
<td>Mn</td>
<td>0.9</td>
<td>5.4</td>
<td>4.0</td>
<td>0.4</td>
<td>0.8</td>
</tr>
<tr>
<td>Fe</td>
<td>2.9</td>
<td>18.8</td>
<td>14.7</td>
<td>1.4</td>
<td>2.8</td>
</tr>
<tr>
<td>Ni</td>
<td>1.0</td>
<td>6.7</td>
<td>5.7</td>
<td>39.1</td>
<td>1.0</td>
</tr>
<tr>
<td>Zr</td>
<td>–</td>
<td>–</td>
<td>11.9</td>
<td>–</td>
<td>39.6</td>
</tr>
<tr>
<td>Mo</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

### Table 2. Comparison of the modified Rc values (RF10+ data) with other evaluations.

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Abundance, %</th>
<th>$\text{Rc, barn}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Atlas-2006</td>
</tr>
<tr>
<td>Cr-50</td>
<td>4.3</td>
<td>1.7 ± 0.2</td>
</tr>
<tr>
<td>Cr-52</td>
<td>83.8</td>
<td>0.48</td>
</tr>
<tr>
<td>Cr-53</td>
<td>9.5</td>
<td>12.3</td>
</tr>
<tr>
<td>Cr-54</td>
<td>2.4</td>
<td>0.25 ± 0.04</td>
</tr>
<tr>
<td>Cr-nat</td>
<td>–</td>
<td>2.1 ± 0.2</td>
</tr>
<tr>
<td>Mn-55</td>
<td>100.0</td>
<td>13.4 ± 0.5</td>
</tr>
<tr>
<td>Fe-54</td>
<td>5.8</td>
<td>1.27 ± 0.10</td>
</tr>
<tr>
<td>Fe-56</td>
<td>91.8</td>
<td>1.36 ± 0.15</td>
</tr>
<tr>
<td>Fe-57</td>
<td>2.1</td>
<td>1.51 ± 0.15</td>
</tr>
<tr>
<td>Fe-58</td>
<td>0.3</td>
<td>1.50 ± 0.07</td>
</tr>
<tr>
<td>Fe-nat</td>
<td>–</td>
<td>1.32</td>
</tr>
<tr>
<td>Ni-58</td>
<td>68.1</td>
<td>2.1 ± 0.2</td>
</tr>
<tr>
<td>Ni-60</td>
<td>26.2</td>
<td>1.4 ± 0.2</td>
</tr>
<tr>
<td>Ni-61</td>
<td>1.1</td>
<td>2.1 ± 0.4</td>
</tr>
<tr>
<td>Ni-62</td>
<td>7.3</td>
<td>6.85 ± 0.36</td>
</tr>
<tr>
<td>Ni-64</td>
<td>0.9</td>
<td>1.07 ± 0.15</td>
</tr>
<tr>
<td>Ni-nat</td>
<td>–</td>
<td>2.07</td>
</tr>
<tr>
<td>Zr-90</td>
<td>51.4</td>
<td>0.17 ± 0.02</td>
</tr>
<tr>
<td>Zr-91</td>
<td>11.2</td>
<td>5.76 ± 0.40</td>
</tr>
<tr>
<td>Zr-92</td>
<td>17.2</td>
<td>0.64</td>
</tr>
<tr>
<td>Zr-94</td>
<td>17.4</td>
<td>0.28 ± 0.01</td>
</tr>
<tr>
<td>Zr-96</td>
<td>2.8</td>
<td>5.28 ± 0.11</td>
</tr>
<tr>
<td>Zr-nat</td>
<td>–</td>
<td>1.10 ± 0.15</td>
</tr>
</tbody>
</table>

### 3. Benchmarks selection for modified data testing

The modified files of neutron data were tested on the benchmark models selected from the ICSBEP Handbook. All selected experiments are critical assemblies with intermediate or fast neutron spectrum. Also selected were simple models in spherical geometry with reflectors of different thicknesses. The structural materials are used as a reflector for most models, but for some models – both as a reflector material, and as a load of the core. Selected experiments can be divided into five groups (lists) in accordance with their characteristics.

List 1: KBR experiments for testing capture cross sections of structural materials.

List 2: Experiments on the compact critical assemblies with iron reflectors for testing the neutron angular distribution anisotropy of the elastic scattering on Fe:

– PMF-015, PMF-025, PMF-026, PMF-028, PMF-032;
– HMF-013, HMF-021, HMF-084/7, HMF-084/19.

List 3: Experiments containing a large amount of SS or Fe in the core with SS reflectors for testing the total effect of anisotropy in the elastic scattering and neutron capture in Fe:

– PMI-002 (ZPR-6/10) and HMI-001 (ZPR-9/34).

List 4: Experiments with Mo and Fe (as a major neutron absorbers in the KBR-10 assembly). Neutron data for Mo have not been revised. However, to identify the trends and possible future modifications of neutron cross sections by testing the Mo data, the critical assemblies with Mo were also selected:

– PMF-044/1 and HCM-003.

List 5: Experiments with Ni reflector:

– PMF-014, HMF-003/12, HMF-084/10, HMF-084/22, and MCF-004 (ZPR-3/56B).

Critical experiments highly sensitive to neutron data of Zr at intermediate or fast energy range were not found.

### 4. Code used for calculations of criticality

The MCNP5 code [9] was used for calculation of criticality of different benchmark models.

### 5. Neutron data libraries used

In addition to the RF10 and RF10+ libraries, the following evaluated neutron data were used in the...
calculations: ENDF/B-VII.1 (E-71), ENDF/B-VIIIbeta1 (E-8b1), JENDL-4.0 (JL40), JEFF-3.2 (JF32). The library abbreviations used further for references are given in parentheses.

The neutron data for calculations with files from RF10, RF10+, JL40 and E-8b1 libraries were prepared using the NJOY2012 code [10]. Neutron data in the ACE format for the E-71 library were taken from the web-site [11], and for JF32 the data were obtained from the NEA Data Bank.

6. Results of testing

The following designations are used below: E means the experimental (evaluated) benchmark value and C – the calculated value.

Testing of the modified neutron data for structural materials was carried out in two steps. First, the calculations of \( k_{\infty} \) values for the KBR benchmark models sensitive to the capture cross section of testing materials were performed (List 1). Because the original evaluation of \( k_{\infty} \) model values for HCI-005 benchmarks was performed on the basis of the ABBN-93 group constants library [12] the results of C/E-1 differences of \( k_{\infty} \) values for ABBN93 library are also shown in Fig. 1 (ABBN93).

Figure 1 shows that the use of modified data RF10+ leads to a significant decrease in the difference between the calculated and experimental results. Comparison of calculational results for the benchmark models with Mo and Zr show a reduction in the capture cross section for both materials.

The neutron data for calculations with files from RF10, RF10+, JL40 and E-8b1 libraries were prepared using the NJOY2012 code [10]. Neutron data in the ACE format for the E-71 library were taken from the web-site [11], and for JF32 the data were obtained from the NEA Data Bank.

6. Results of testing

The following designations are used below: E means the experimental (evaluated) benchmark value and C – the calculated value.

Testing of the modified neutron data for structural materials was carried out in two steps. First, the calculations of \( k_{\infty} \) values for the KBR benchmark models sensitive to the capture cross section of testing materials were performed (List 1). Because the original evaluation of \( k_{\infty} \) model values for HCI-005 benchmarks was performed on the basis of the ABBN-93 group constants library [12] the results of C/E-1 differences of \( k_{\infty} \) values for ABBN93 library are also shown in Fig. 1 (ABBN93).

Figure 1 shows that the use of modified data RF10+ leads to a significant decrease in the difference between the calculated and experimental results. Comparison of calculational results for the benchmark models with Mo and Zr show a reduction in the capture cross section for both materials.

The neutron data for calculations with files from RF10, RF10+, JL40 and E-8b1 libraries were prepared using the NJOY2012 code [10]. Neutron data in the ACE format for the E-71 library were taken from the web-site [11], and for JF32 the data were obtained from the NEA Data Bank.

6. Results of testing

The following designations are used below: E means the experimental (evaluated) benchmark value and C – the calculated value.

Testing of the modified neutron data for structural materials was carried out in two steps. First, the calculations of \( k_{\infty} \) values for the KBR benchmark models sensitive to the capture cross section of testing materials were performed (List 1). Because the original evaluation of \( k_{\infty} \) model values for HCI-005 benchmarks was performed on the basis of the ABBN-93 group constants library [12] the results of C/E-1 differences of \( k_{\infty} \) values for ABBN93 library are also shown in Fig. 1 (ABBN93).

Figure 1 shows that the use of modified data RF10+ leads to a significant decrease in the difference between the calculated and experimental results. Comparison of calculational results for the benchmark models with Mo and Zr show a reduction in the capture cross section for both materials.

The neutron data for calculations with files from RF10, RF10+, JL40 and E-8b1 libraries were prepared using the NJOY2012 code [10]. Neutron data in the ACE format for the E-71 library were taken from the web-site [11], and for JF32 the data were obtained from the NEA Data Bank.

6. Results of testing

The following designations are used below: E means the experimental (evaluated) benchmark value and C – the calculated value.

Testing of the modified neutron data for structural materials was carried out in two steps. First, the calculations of \( k_{\infty} \) values for the KBR benchmark models sensitive to the capture cross section of testing materials were performed (List 1). Because the original evaluation of \( k_{\infty} \) model values for HCI-005 benchmarks was performed on the basis of the ABBN-93 group constants library [12] the results of C/E-1 differences of \( k_{\infty} \) values for ABBN93 library are also shown in Fig. 1 (ABBN93).

Figure 1 shows that the use of modified data RF10+ leads to a significant decrease in the difference between the calculated and experimental results. Comparison of calculational results for the benchmark models with Mo and Zr show a reduction in the capture cross section for both materials.

The neutron data for calculations with files from RF10, RF10+, JL40 and E-8b1 libraries were prepared using the NJOY2012 code [10]. Neutron data in the ACE format for the E-71 library were taken from the web-site [11], and for JF32 the data were obtained from the NEA Data Bank.

6. Results of testing

The following designations are used below: E means the experimental (evaluated) benchmark value and C – the calculated value.

Testing of the modified neutron data for structural materials was carried out in two steps. First, the calculations of \( k_{\infty} \) values for the KBR benchmark models sensitive to the capture cross section of testing materials were performed (List 1). Because the original evaluation of \( k_{\infty} \) model values for HCI-005 benchmarks was performed on the basis of the ABBN-93 group constants library [12] the results of C/E-1 differences of \( k_{\infty} \) values for ABBN93 library are also shown in Fig. 1 (ABBN93).

Figure 1 shows that the use of modified data RF10+ leads to a significant decrease in the difference between the calculated and experimental results. Comparison of calculational results for the benchmark models with Mo and Zr show a reduction in the capture cross section for both materials.
Table 4. C/E-1 differences in $k_{\text{eff}}$ values for benchmark model containing molybdenum (list 4).

<table>
<thead>
<tr>
<th>ID</th>
<th>dE, %</th>
<th>C/E-1, %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>E-71</td>
<td>JF32</td>
</tr>
<tr>
<td>PMF-044/1</td>
<td>0.21</td>
<td>-0.15</td>
</tr>
<tr>
<td>HCM-003/1</td>
<td>0.20</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Table 5. C/E-1 differences in $k_{\text{eff}}$ values for models with nickel reflectors of varying thickness T (list 5).

<table>
<thead>
<tr>
<th>T, cm</th>
<th>ID</th>
<th>dE, %</th>
<th>C/E-1, %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>E-71</td>
<td>JF32</td>
<td>JL40</td>
</tr>
<tr>
<td>1.27</td>
<td>HMF-084/22</td>
<td>0.20</td>
<td>-0.40</td>
</tr>
<tr>
<td>2.54</td>
<td>HMF-084/10</td>
<td>0.22</td>
<td>0.16</td>
</tr>
<tr>
<td>3.02</td>
<td>HMF-003/12</td>
<td>0.10</td>
<td>0.08</td>
</tr>
<tr>
<td></td>
<td>MCF-004</td>
<td>0.31</td>
<td>0.19</td>
</tr>
<tr>
<td></td>
<td>PMF-014</td>
<td>-0.11</td>
<td>0.11</td>
</tr>
</tbody>
</table>

the possibility of reducing the Mo capture cross-section. It is consistent with the result of the calculation $k_\infty$ on KBR-10 assembly.

The results of testing Ni neutron data are presented in Table 5 (List 5). Data in the table are given depending on the reflector thickness T.

The comparison of the results shows that the use of RF10+ data leads to the consistency for PMF-014 and MCF-004 benchmark models, but did not improve the agreement for simple spherical systems with a reflector made of Ni. It should be noted that the dependence of C/E-1 on the reflector thickness is similar for simple spherical systems for all libraries, as it was indicated in Ref. [5]. This can be due to the crude description of the energy dependence of the anisotropy in the elastic neutron scattering angular distributions.

7. Conclusion

Using of the modified nuclear data of Cr, Mn, Fe, Ni, and Zr structural materials from the RF10+ neutron data library leads to significant improvement of the C/E ratio for the KBR assemblies. Significant improvement of agreement between the calculated and evaluated values for the benchmarks with Fe reflectors was also observed.

The C/E results obtained with the RF10+ library for complex benchmark models highly sensitive to the cross sections of structural materials show that they are no worse than the results obtained with other evaluated data libraries.

Possible improvement in results by decreasing the capture cross section for Zr and Mo at the energies above 1 keV is indicated.

References

[1] International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA n° 7281, NEA/NSC(95)/03, September 2015 edition