EPJ Web of Conferences **111**, 11005 (2016)
DOI: 10.1051/epjconf/201611111005


# Validation of the BUGJEFF311.BOLIB, BUGENDF70.BOLIB and BUGLE-B7 broad-group libraries on the PCA-Replica ($H_2O$/Fe) neutron shielding benchmark experiment

Massimo Pescarini[a], Roberto Orsi and Manuela Frisoni

*ENEA, CR "E. Clementel", Via Martiri di Monte Sole 4, 40129 Bologna, Italy*

**Abstract.** The PCA-Replica 12/13 ($H_2O$/Fe) neutron shielding benchmark experiment was analysed using the TORT-3.2 3D $S_N$ code. PCA-Replica reproduces a PWR ex-core radial geometry with alternate layers of water and steel including a pressure vessel simulator. Three broad-group coupled neutron/photon working cross section libraries in FIDO-ANISN format with the same energy group structure (47 n + 20 γ) and based on different nuclear data were alternatively used: the ENEA BUGJEFF311.BOLIB (JEFF-3.1.1) and BUGENDF70.BOLIB (ENDF/B-VII.0) libraries and the ORNL BUGLE-B7 (ENDF/B-VII.0) library. Dosimeter cross sections derived from the IAEA IRDF-2002 dosimetry file were employed. The calculated reaction rates for the Rh-103(n,n')Rh-103m, In-115(n,n')In-115m and S-32(n,p)P-32 threshold activation dosimeters and the calculated neutron spectra are compared with the corresponding experimental results.

## 1 Introduction

ENEA-Bologna analysed the PCA-Replica 12/13 [1] water/iron ($H_2O$/Fe) low-flux engineering neutron shielding benchmark experiment included in the OECD-NEADB/ORNL-RSICC NEA-1517 SINBAD database. Three-dimensional (3D) fixed source transport calculations were performed through the TORT-3.2 [2,3] discrete ordinates ($S_N$) code. PCA-Replica reproduces a PWR ex-core radial geometry and is particularly suitable to test the cross section libraries specifically dedicated to LWR shielding and pressure vessel dosimetry applications. Two ENEA-Bologna freely released (at OECD-NEADB and ORNL-RSICC) broad-group libraries named NEA-1866 BUGJEFF311.BOLIB [4] and NEA-1872 BUGENDF70.BOLIB [5], respectively based on the OECD-NEADB JEFF-3.1.1 [6,7] and US ENDF/B-VII.0 [8] evaluated nuclear data libraries, were alternatively used together with the ORNL BUGLE-B7 [9] similar library based on ENDF/B-VII.0 data. All these libraries, dedicated to the previously cited applications, include parameterized sets of problem-dependent self-shielded neutron cross sections specifically prepared for BWR and PWR applications, adopt the FIDO-ANISN format and have the same broad-group coupled neutron/photon energy group structure (47 n + 20 γ) as the older ORNL BUGLE-96 [10] library. The ENEA libraries were obtained through problem-dependent cross section collapsing from their ENEA fine-group mother libraries with a nuclear data processing methodology similar to that adopted to generate BUGLE-96, using in particular the same compositional, geometrical and temperature input data to perform the cross section collapsing. BUGJEFF311.BOLIB and BUGENDF70.BOLIB were in fact respectively obtained from the NEA-

[a] Corresponding author: massimo.pescarini@enea.it

1869 VITJEFF311.BOLIB [11] and NEA-1870 VITENDF70.BOLIB [12] fine-group libraries in AMPX format for nuclear fission applications through problem-dependent cross section collapsing with the ENEA-Bologna 2007 revision [13] of the ORNL SCAMPI [14] nuclear data processing system. Both previous libraries are based on the Bondarenko [15] self-shielding factor method, were generated through the LANL NJOY-99.259 nuclear data processing system and have the same fine-group energy structure (199 n + 42 $\gamma$) as the ORNL VITAMIN-B6 [10] and VITAMIN-B7 [9] similar libraries from which BUGLE-96 and BUGLE-B7 were respectively obtained. It is underlined that, differently from the ENEA libraries, VITAMIN-B7 and BUGLE-B7 were generated through the recent ORNL AMPX-6.1 nuclear data processing system not yet freely distributed. In the present work the PCA-Replica calculated neutron dose and spectrum integral results, obtained using the three cited working libraries, are compared with the corresponding experimental data.

## 2 The PCA-Replica experimental facility and measurements

The PCA-Replica (Winfrith, UK, 1984) experimental facility duplicated exactly the ex-core radial geometry of the ORNL PCA (Poo1 Critical Assembly) similar experiment (Oak Ridge, US, 1981), simulating the ex-core radial geometry of a PWR. PCA-Replica reproduces the 12/13 configuration of PCA with a first water gap of about 12 cm between the core and a thermal shield (TS) simulator and a second water gap of about 13 cm between TS and a PWR pressure vessel (RPV) simulator. The PCA low-flux reactor neutron source was replaced in PCA-Replica with a neutron source emitted by a thin fission plate with the same rectangular cross-sectional area of the PCA reactor source. This simpler source configuration could more easily be calibrated with a high degree of accuracy with respect to the PCA reactor source. The parallelepiped fission plate (63.5 $\times$ 40.2 $\times$ 0.6 cm) was made of highly enriched uranium (93.0 w% in U-235) alloyed with aluminium. It was irradiated by the NESTOR reactor (30 kW at the maximum power) through a graphite thermal column (total thickness = 43.91 cm) in the ASPIS shielding facility. Beyond the fission plate (0.6 cm thick), the PCA-Replica shielding array was arranged in a large parallelepiped steel tank (square section; side 180.0 cm) filled with water and surrounded by a thick concrete shield. After the first water gap (12.1 cm thick) there was the stainless steel TS simulator (5.9 cm thick), the second water gap (12.7 cm thick) and the mild steel RPV simulator (thickness T = 22.5 cm) tightly connected with a void box made of a thin layer (0.3 cm thick) of aluminium, simulating the air cavity (29.58 cm thick) between the RPV and the biological shield in a PWR. All these components were perfectly orthogonally aligned and centred along the Z horizontal axis passing through the centroid of the fission plate. Threshold activation neutron dosimeters and neutron spectrometers were located in all or in part of the ten measurement spatial positions along the Z axis. The Rh-103(n,n')Rh-103m, In-115(n,n')In-115m and S-32(n,p)P-32 dosimeters employed are respectively characterized by the effective energy thresholds 0.69, 1.30 and 2.70 MeV, by the median energies 1.9, 2.4 and 3.9 MeV and by the 90% response energy ranges 0.53 - 5.4 MeV, 1.0 - 5.6 MeV and 2.2 - 7.4 MeV. The spectral measurements were performed only in two positions (1/4 T RPV and void box) with two kinds of spectrometer. The spherical hydrogen-filled proportional counters of type SP-2 were used in combination, to cover the energy range from 50.0 keV to 1.2 MeV. The neutron fluxes between 1.0 and 10.0 MeV were determined with a spherical 3.5 ml organic liquid (NE213) scintillator.

## 3 Transport calculations

The whole PCA-Replica experimental array was reproduced in Cartesian (X,Y,Z) geometry (see Figure 1) with the TORT-3.2 code to assure a detailed description of the spatial inhomogeneity of the neutron source emitted by the fission plate. The NEA-1708 ADEFTA-4.1 [16] program calculated the isotopic atomic densities from the isotopic abundances reported in the BNL-NNDC database. The automatic spatial mesh generation and the graphical verification of the geometrical model were performed through the NEA-1678/09 BOT3P-5.3 [17,18] pre/post-processor system.

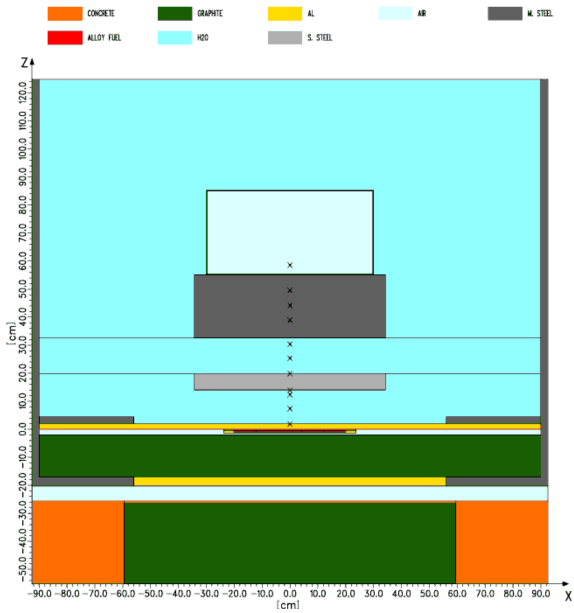


**Figure 1.** PCA-Replica - Geometrical and compositional model horizontal section at Y = 0. cm, dosimeter locations “×”, TORT-3.2 (X,Y,Z) with 65X×63Y×182Z spatial meshes.

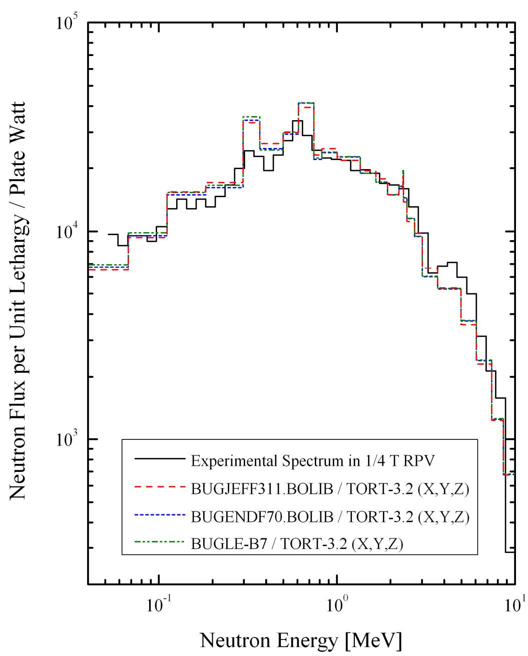


**Figure 2.** PCA-Replica - Comparison of experimental and calculated neutron spectra in mild steel, in the 1/4 T RPV measurement position at Z = 39.01 cm.

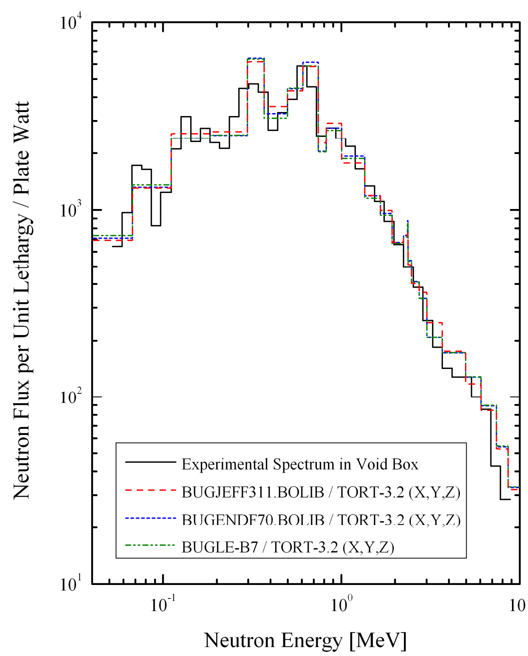


**Figure 3.** PCA-Replica - Comparison of experimental and calculated neutron spectra in air, in the void box measurement position at Z = 58.61 cm.

**Table 1.** PCA-Replica - Summary of Experimental (E) and Calculated (C) Rh-103(n,n'), In-115(n,n') and S-32(n,p) reaction rates[a] per NESTOR reactor Watt along the horizontal axis Z.

| Dos. Pos. | Distance from Fission Plate on the Axis Z [cm] | Experimental Reaction Rate[a] ± Random Error (1σ) (E) | BUGJEFF311. BOLIB Calculation | | BUGENDF70. BOLIB Calculation | | BUGLE-B7 Calculation | | Reference Location |
|---|---|---|---|---|---|---|---|---|---|
| | | | Calculated Reaction Rate[a] (C) | C/E[b] | Calculated Reaction Rate[a] (C) | C/E[b] | Calculated Reaction Rate[a] (C) | C/E[b] | |
| Rh-103(n,n')Rh-103m<br>Systematic Error = ± 3.0% in All Dosimeter Measurement Positions | | | | | | | | | |
| 1 | 1.91 | 1.69E-20 ± 3.0% | 1.81E-20 | 1.09 | 1.81E-20 | 1.09 | 1.82E-20 | 1.10 | 12 cm Water Gap 1 |
| 2 | 7.41 | 3.78E-21 ± 3.0% | 3.43E-21 | 0.93 | 3.44E-21 | 0.93 | 3.46E-21 | 0.93 | |
| 3 | 12.41 | 1.40E-21 ± 3.0% | 1.30E-21 | 0.95 | 1.31E-21 | 0.95 | 1.32E-21 | 0.96 | |
| 4 | 14.01 | 1.27E-21 ± 3.0% | 1.15E-21 | 0.93 | 1.16E-21 | 0.93 | 1.17E-21 | 0.94 | |
| 5 | 19.91 | 4.23E-22 ± 3.0% | 4.18E-22 | 1.01 | 4.17E-22 | 1.00 | 4.16E-22 | 1.00 | 13 cm Water Gap 2 |
| 6 | 25.41 | 1.15E-22 ± 4.0% | 1.02E-22 | 0.91 | 1.02E-22 | 0.91 | 1.03E-22 | 0.91 | |
| 7 | 30.41 | 4.73E-23 ± 4.0% | 4.12E-23 | 0.89 | 4.13E-23 | 0.89 | 4.15E-23 | 0.89 | |
| 8 | 39.01 | 2.07E-23 ± 1.0% | 2.02E-23 | 1.02 | 2.02E-23 | 1.01 | 2.02 E-23 | 1.02 | 1/4 T RPV |
| 9 | 49.61 | 5.53E-24 ± 1.9% | 5.62E-24 | 1.06 | 5.59E-24 | 1.05 | 5.56E-24 | 1.05 | 3/4 T RPV |
| 10 | 58.61 | 1.80E-24 ± 1.6% | 1.65E-24 | 0.96 | 1.66E-24 | 0.96 | 1.62E-24 | 0.94 | Void Box |
| In-115(n,n')In-115m<br>Systematic Error = ± 2.0% in All Dosimeter Measurement Positions | | | | | | | | | |
| 8 | 39.01 | 3.93E-24 ± 0.9% | 3.89E-24 | 1.03 | 3.87E-24 | 1.03 | 3.88E-24 | 1.03 | 1/4 T RPV |
| 9 | 49.61 | 8.23E-25 ± 1.4% | 7.80E-25 | 0.99 | 7.76E-25 | 0.98 | 7.70E-25 | 0.97 | 3/4 T RPV |
| 10 | 58.61 | 2.31E-25 ± 1.5% | 2.15E-25 | 0.97 | 2.16E-25 | 0.97 | 2.12E-25 | 0.95 | Void Box |
| S-32(n,p)P-32<br>Systematic Error = ± 4.0% in All Dosimeter Measurement Positions | | | | | | | | | |
| 8 | 39.01 | 1.08E-24 ± 1.5% | 9.86E-25 | 0.95 | 9.78E-25 | 0.94 | 9.83E-25 | 0.95 | 1/4 T RPV |
| 9 | 49.61 | 1.46E-25 ± 1.9% | 1.38E-25 | 0.98 | 1.35E-25 | 0.97 | 1.36E-25 | 0.97 | 3/4 T RPV |
| 10 | 58.61 | 3.73E-26 ± 1.3% | 3.63E-26 | 1.01 | 3.57E-26 | 1.00 | 3.57E-26 | 1.00 | Void Box |

Note: Total experimental error (1σ confidence level) = $[(\text{random error})^2 + (\text{systematic error})^2]^{1/2}$ (see [1]).

([a]) Reaction rates are in units of reactions × $s^{-1}$× $atom^{-1}$ × NESTOR $Watt^{-1}$.

([b]) Experimental results contain a contribution from the NESTOR core background. Calculated results refer only to the neutrons produced in the fission plate per 1 Watt of NESTOR power. The E values, in the C/E ratios, are reduced by 4% in the RPV and void box and by 2% in the water gaps (see [1]).

A parallelepiped geometry (185.08 × 180.0 × 180.0 cm, respectively along the X, Y and Z axis) was described with a 65X×63Y×182Z fine spatial mesh grid. Volumetric meshes with sides always inferior to 0.5 cm were introduced to get the best result accuracy in the measurement positions on the Z axis. Group-organized files of macroscopic cross sections, requested by TORT-3.2, were prepared through the GIP [4] program. Fixed source transport calculations with one source (outer) iteration were performed using fully symmetrical discrete ordinates directional quadrature sets for the flux solution. The $P_3$-$S_8$ approximation, adopted in all the calculations, is the most widely used option in fixed source calculations for LWR safety analyses. $P_N$ corresponds to the order of the expansion in Legendre polynomials of the scattering cross section matrix and $S_N$ represents the order of the flux angular discretization. The same value (1.0E-03) for the point-wise flux convergence criterion was employed. The vacuum boundary condition was selected at the left, right, inside, outside, bottom and top geometrical boundaries. The same set of flat weighting dosimeter cross sections for Rh-103(n,n'), In-115(n,n') and S-32(n,p), derived from the IAEA International Reactor Dosimetry File IRDF-2002, was used in all the calculations. The volumetric neutron sources used in the calculations with the three libraries were got using their own U-235 fission neutron spectra whereas the common value of $\overline{\nu}$ (U-235) = 2.437 [1] for the average number of neutrons produced per U-235 thermal fission was used in all the calculations to assure a consistent result intercomparison. The value of 6.74E-04 fission plate Watts per NESTOR Watt [1] was given to the source multiplier parameter for the neutron source. The calculated/experimental dosimetric results are reported in Table 1. The calculated/experimental spectra in the 1/4 T RPV and void box positions are respectively shown in Figures 2 and 3.

## 4 Conclusion

The deviations of the dosimetric results from the corresponding experimental ones are within the desired ± 10-15% target accuracy. Given that the total experimental uncertainty ranges from about 2% to a maximum of 5% (1σ), then the calculated results exhibit very good statistical consistency with the corresponding measurements. The results obtained using BUGENDF70.BOLIB and BUGLE-B7 are very similar and this seems to indicate an equivalent performance of the NJOY-99.259/SCAMPI and AMPX-6.1 nuclear data processing calculation chains starting from the same ENDF/B-VII.0 data.

## References

1. J. Butler et al., UKAEA, AEE Winfrith Report AEEW-R 1736 (January 1984)
2. W.A. Rhoades, D.B. Simpson, TORT Version 3, ORNL/TM-13221 (October 1997)
3. DOORS3.1, ORNL, RSIC CCC-650 (August 1996)
4. M. Pescarini, V. Sinitsa , R.Orsi, M. Frisoni, ENEA Int. Report UTFISSM-P9H6-2 Rev.1 (2013)
5. M. Pescarini, V. Sinitsa , R.Orsi, M. Frisoni, ENEA Int. Report UTFISSM-P9H6-8 (2013)
6. *The JEFF-3.1.1 Nuclear Data Library*, JEFF Report 22, OECD-NEA Data Bank (2009)
7. *The JEFF-3.1 Nuclear Data Library*, JEFF Report 21, OECD-NEA Data Bank (2006)
8. M.B. Chadwick et al., Nucl. Data Sheets, **107**, 12, pp. 2931-3060, (December 2006)
9. J.M. Risner et al., ORNL/TM-2011/12, NUREG/CR-7045 (September 2011)
10. J.E. White et al., ORNL-6795/R1, NUREG/CR-6214, Revision 1 (January 1995)
11. M. Pescarini, V. Sinitsa, R. Orsi, ENEA Int. Report UTFISSM-P9H6-003 Rev.1 (2011)
12. M. Pescarini, V. Sinitsa, R. Orsi, M. Frisoni, ENEA Int. Report UTFISSM-P9H6-005 (2012)
13. V. Sinitsa, M. Pescarini, ENEA Int. Report FPN-P9H6-006 (2007)
14. SCAMPI, ORNL, RSIC PSR-352 (September 1995)
15. I.I. Bondarenko et al., *Group constants for nuclear reactors calculations* (Cons. Bureau, 1964)
16. R. Orsi, ENEA Int. Report FPN-P9H6-10 (2008)
17. R. Orsi, ENEA Int. Report FPN-P9H6-11 (2008)
18. R. Orsi, Nuc. Sci. and Eng., Technical Note, **146**, pp. 248-255 (2004)