

**Titolo**

# Three-Dimensional (X,Y,Z) Deterministic Analysis of the PCA-Replica Neutron Shielding Benchmark Experiment Using the TORT-3.2 Code and Group Cross Section Libraries for LWR Shielding and Pressure Vessel Dosimetry

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**Sommario**

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**Note**

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# Three-dimensional (X,Y,Z) deterministic analysis of the PCA-Replica neutron shielding benchmark experiment using the TORT-3.2 code and group cross section libraries for LWR shielding and pressure vessel dosimetry

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**Abstract.** The PCA-Replica 12/13 (H<sub>2</sub>O/Fe) neutron shielding benchmark experiment was analysed using the ORNL TORT-3.2 3D S<sub>N</sub> code. PCA-Replica, specifically conceived to test the accuracy of nuclear data and transport codes employed in LWR shielding and radiation damage calculations, reproduces a PWR ex-core radial geometry with alternate layers of water and steel including a PWR 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  $\gamma$ ) 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-96 (ENDF/B-VI.3) 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

The ENEA-Bologna Nuclear Data Group analysed the PCA-Replica 12/13 [1] water/iron (H<sub>2</sub>O/Fe) low-flux engineering neutron shielding benchmark experiment included in the SINBAD [2] international database. Three-dimensional (3D) fixed source transport calculations in Cartesian geometry through the TORT-3.2 [3] discrete ordinates (S<sub>N</sub>) code, included in the ORNL DOORS [4] system of deterministic transport codes, were performed. 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 multi-group libraries named BUGJEFF311.BOLIB [5] and BUGENDF70.BOLIB [6], respectively based on the OECD-NEADB JEFF-3.1.1 [7, 8] and US ENDF/B-VII.0 [9] evaluated nuclear data libraries, were alternatively used in the calculations together with the ORNL BUGLE-96 [10] similar library based on ENDF/B-VI.3 data. In particular BUGLE-96, internationally widely used with success for a long time, was assumed as a reliable reference standard to test the ENEA libraries. All the cited libraries dedicated to the mentioned applications include parameterized sets of problem-dependent self-shielded neutron cross sections specifically prepared for BWR and PWR applications,

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adopt the FIDO-ANISN format and have the same broad-group coupled ( $47 n + 20 \gamma$ ) neutron/photon energy group structure. They were obtained through problem-dependent cross section collapsing from their fine-group mother libraries with a similar nuclear data processing methodology using in particular the same compositional, geometrical and temperature input data (see [11]) to perform the cross section collapsing. In particular the BUGJEFF311.BOLIB and BUGENDF70.BOLIB libraries were respectively obtained from the ENEA-Bologna VITJEFF311.BOLIB [12] and VITENDF70.BOLIB [13] fine-group libraries in AMPX format for nuclear fission applications through problem-dependent cross section collapsing with the ENEA-Bologna 2007 revision [14] of the ORNL SCAMPI [15] nuclear data processing system. Both previous libraries are based on the Bondarenko [16] self-shielding factor method and have the same fine-group energy structure ( $199 n + 42 \gamma$ ) as the ORNL VITAMIN-B6 [10] similar library from which BUGLE-96 was obtained at ORNL. The ENEA-Bologna programs ADEFTA-4.1 [17] and BOT3P-5.3 [18, 19] were respectively employed for the calculation of the isotopic atomic densities and for the automatic generation of the spatial mesh grid of the geometrical model. The calculated neutron dose and spectrum integral results were compared with the corresponding experimental data (see [20]), respectively obtained using three types of threshold activation dosimeters and two kinds of spectrometer. The dosimeter neutron cross section sets used in the calculations were derived (see [21]) from the IAEA IRDF-2002 [22] international reactor dosimetry file.

## 2 The PCA-Replica experimental facility and measurements

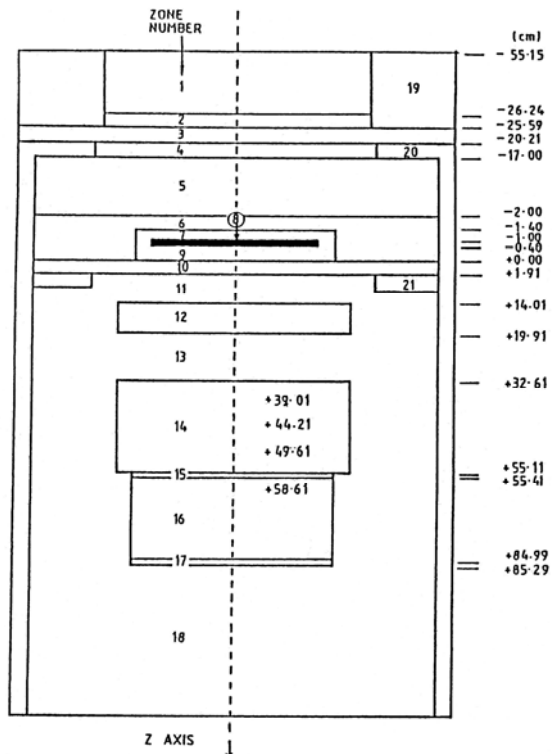
The PCA-Replica (Winfrith, UK, 1984) experimental facility duplicated exactly the ex-core radial geometry of the ORNL PCA (Pool Critical Assembly) [23] similar experiment (Oak Ridge, US, 1981), simulating the ex-core radial geometry of a PWR. In particular PCA-Replica reproduces the 12/13 configuration of the PCA experiment with a water gap of about 12 cm between the core and a PWR thermal shield (TS) simulator and a water gap of about 13 cm between the 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, reducing a possible cause of the in-vessel neutron flux underestimations noted in transport analyses dedicated to PCA, despite the extensive work addressed to obtain an accurate calibration [24]. 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 (see Figure 1). 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 imaginary line Z (horizontal or nuclear 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 [25] 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 and discussion of the results

The whole PCA-Replica experimental array (see [1] and Figures 1 and 2) was reproduced in the Cartesian (X,Y,Z) geometry with the TORT-3.2 code to assure first of all an accurate detailed description of the spatial inhomogeneity of the neutron source emitted by the fission plate. The ADEFTA-4.1 program was employed in the calculation of the isotopic atomic densities on the basis of the atomic abundances reported in the BNL-NNDC database [26] included in ADEFTA. The automatic spatial mesh generation and the graphical verification of the geometrical model were performed through the BOT3P-5.3 pre/post-processor system. It was described a parallelepiped geometry ( $185.08 \times 180.0 \times 180.0$  cm, respectively along the X, Y and Z axis) with a  $65X \times 63Y \times 182Z$  fine spatial mesh grid. Volumetric meshes with sides always inferior to 0.5 cm were introduced to obtain the best result accuracy along the Z horizontal axis where the experimental measurement positions were located. The BUGJEFF311.BOLIB, BUGENDF70.BOLIB and BUGLE-96 libraries were alternatively used in the calculations. Both infinite dilution and self-shielded cross sections were selected. Self-shielded cross sections from the three library packages were used when available. It is underlined that the stainless steel TS and the mild steel RPV simulators of PCA-Replica were characterized by atomic densities quite similar to those used to determine the background cross sections employed in the self-shielding of the BUGJEFF311.BOLIB, BUGENDF70.BOLIB and BUGLE-96 neutron cross sections. Group-organized files of macroscopic cross sections, requested by TORT-3.2, were prepared through the ORNL GIP (see [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 was adopted as the standard reference.  $P_N$  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. It is underlined that the  $P_3$ - $S_8$  approximation is the most widely used option in the fixed source calculations dedicated to LWR safety analyses. A further parametric analysis, using exclusively BUGJEFF311.BOLIB, was performed on the  $P_N$  and  $S_N$  orders.  $P_3$  and  $P_5$  calculations were performed with different sets of fully symmetrical quadrature:  $P_3$ - $S_8$ ,  $P_3$ - $S_{12}$ ,  $P_3$ - $S_{16}$ ,  $P_5$ - $S_{12}$  and  $P_5$ - $S_{16}$ . 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 the Rh-103(n,n')Rh-103m, In-115(n,n')In-115m and S-32(n,p)P-32 nuclear reactions derived (see [16]) from IRDF-2002 was used for the water and steel experimental measurement positions in the calculations with all working libraries. Three different sets of 1/4 T RPV weighting dosimeter cross sections derived (see [16]) from IRDF-2002, singularly included in each package of the three working libraries, were used in addition in the calculations for the steel measurement positions (1/4 T RPV and 3/4 T RPV).

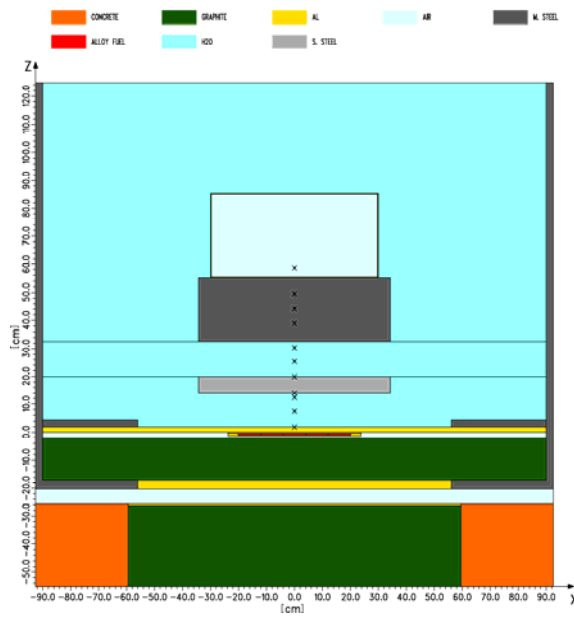
The inhomogeneous spatial distribution (see [1]) of the fission neutron source emitted by the fission plate was employed. The distributed (or volumetric) fission neutron sources used in the calculations with BUGJEFF311.BOLIB, BUGENDF70.BOLIB and BUGLE-96 were obtained using respectively their corresponding U-235 fission neutron spectrum. In order to determine the volumetric neutron source for each working library, the common value of  $\bar{\nu}(U-235) = 2.437$  (see [1]) for the average number of neutrons produced per U-235 thermal fission was used in order to assure a consistent result intercomparison. The value of  $6.74E-04$  fission plate Watts per NESTOR Watt (see [1]) was given to the source multiplier parameter for the inhomogeneous neutron source.

All the dosimetric and spectral results reported herewith refer to TORT-3.2 calculations in  $P_3$ - $S_8$  approximation using the inhomogeneous fission neutron source. Concerning the dosimetric results obtained with flat weighting cross sections (see Table 1 and Figures 3, 4 and 5), only few calculated results for the Rh-103(n,n') dosimeters, obtained with the three working libraries in the second water gap, present underestimated values slightly outside the range of deviation of  $\pm 10\%$  from the corresponding experimental results. The deviations of the calculated results for the In-115(n,n') and S-32(n,p) dosimeters are always contained within  $\pm 10\%$  the corresponding values of the experimental results, available only in the RPV and void box measurement positions.



Graphite: 1, 5. Aluminium: 2, 4, 7, 9, 10, 15, 17. Void (Air): 3, 6, 16. Alloy Fuel (Fission Plate): 8.  
 Water: 11, 13, 18. Stainless Steel: 12. Mild Steel: 14, 20, 21. Concrete: 19.

**Figure 1.** PCA-Replica - Layout of the 12/13 configuration (see [1]).



**Figure 2.** PCA-Replica - Geometrical and compositional model horizontal section at  $Y = 0$ . cm, dosimeter locations “x”, TORT-3.2 (X,Y,Z) with  $65X \times 63Y \times 182Z$  spatial meshes.

**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<sup>a</sup> per NESTOR reactor Watt along the horizontal axis Z.

| Dos. Pos.  | Distance from Fission Plate on the Axis Z [cm] | Experimental Reaction Rate <sup>a</sup> ± Random Error (1σ)<br>(E) | BUGJEFF311. BOLIB Calculation             |                  | BUGENDF70. BOLIB Calculation              |                  | BUGLE-96 Calculation                      |                  | Reference Location |
|--|--|--|---|------------------|---|------------------|---|------------------|--------------------|
|  |  |  | Calculated Reaction Rate <sup>a</sup> (C) | C/E <sup>b</sup> | Calculated Reaction Rate <sup>a</sup> (C) | C/E <sup>b</sup> | Calculated Reaction Rate <sup>a</sup> (C) | C/E <sup>b</sup> |                    |
| Rh-103(n,n')Rh-103m  |  |  |   |                  |   |                  |   |                  |                    |
| 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             | 3.44E-21                                  | 0.93             |                    |
| 3  | 12.41  | 1.40E-21 ± 3.0%  | 1.30E-21                                  | 0.95             | 1.31E-21                                  | 0.95             | 1.30E-21                                  | 0.95             |                    |
| 4  | 14.01  | 1.27E-21 ± 3.0%  | 1.15E-21                                  | 0.93             | 1.16E-21                                  | 0.93             | 1.15E-21                                  | 0.93             |                    |
| 5  | 19.91  | 4.23E-22 ± 3.0%  | 4.18E-22                                  | 1.01             | 4.17E-22                                  | 1.00             | 4.11E-22                                  | 0.99             | 13 cm Water Gap 2  |
| 6  | 25.41  | 1.15E-22 ± 4.0%  | 1.02E-22                                  | 0.91             | 1.02E-22                                  | 0.91             | 1.01E-22                                  | 0.89             |                    |
| 7  | 30.41  | 4.73E-23 ± 4.0%  | 4.12E-23                                  | 0.89             | 4.13E-23                                  | 0.89             | 4.06E-23                                  | 0.88             |                    |
| 8  | 39.01  | 2.07E-23 ± 1.0%  | 2.02E-23                                  | 1.02             | 2.02E-23                                  | 1.01             | 1.98E-23                                  | 1.00             | 1/4 T RPV          |
| 9  | 49.61  | 5.53E-24 ± 1.9%  | 5.62E-24                                  | 1.06             | 5.59E-24                                  | 1.05             | 5.45E-24                                  | 1.03             | 3/4 T RPV          |
| 10   | 58.61  | 1.80E-24 ± 1.6%  | 1.65E-24                                  | 0.96             | 1.66E-24                                  | 0.96             | 1.59E-24                                  | 0.92             | Void Box           |
| In-115(n,n')In-115m  |  |  |   |                  |   |                  |   |                  |                    |
| 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             | 3.81E-24                                  | 1.01             | 1/4 T RPV          |
| 9  | 49.61  | 8.23E-25 ± 1.4%  | 7.80E-25                                  | 0.99             | 7.76E-25                                  | 0.98             | 7.58E-25                                  | 0.96             | 3/4 T RPV          |
| 10   | 58.61  | 2.31E-25 ± 1.5%  | 2.15E-25                                  | 0.97             | 2.16E-25                                  | 0.97             | 2.09E-25                                  | 0.94             | Void Box           |
| S-32(n,p)P-32  |  |  |   |                  |   |                  |   |                  |                    |
| 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             | 9.67E-25                                  | 0.93             | 1/4 T RPV          |
| 9  | 49.61  | 1.46E-25 ± 1.9%  | 1.38E-25                                  | 0.98             | 1.35E-25                                  | 0.97             | 1.34E-25                                  | 0.95             | 3/4 T RPV          |
| 10   | 58.61  | 3.73E-26 ± 1.3%  | 3.63E-26                                  | 1.01             | 3.57E-26                                  | 1.00             | 3.52E-26                                  | 0.98             | Void Box           |

Note: Total experimental error (1σ confidence level) = [(random error)<sup>2</sup> + (systematic error)<sup>2</sup>]<sup>1/2</sup> (see [1]).

<sup>(a)</sup> Reaction rates are in units of reactions × s<sup>-1</sup> × atom<sup>-1</sup> × NESTOR Watt<sup>-1</sup>.

<sup>(b)</sup> 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]).

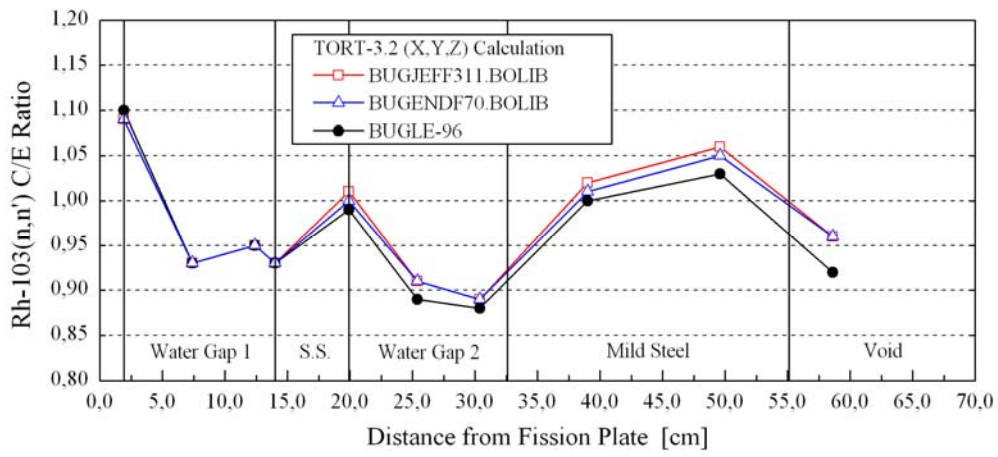


Figure 3. PCA-Replica - Rh-103(n,n') reaction rate ratios (Calculated/Experimental).

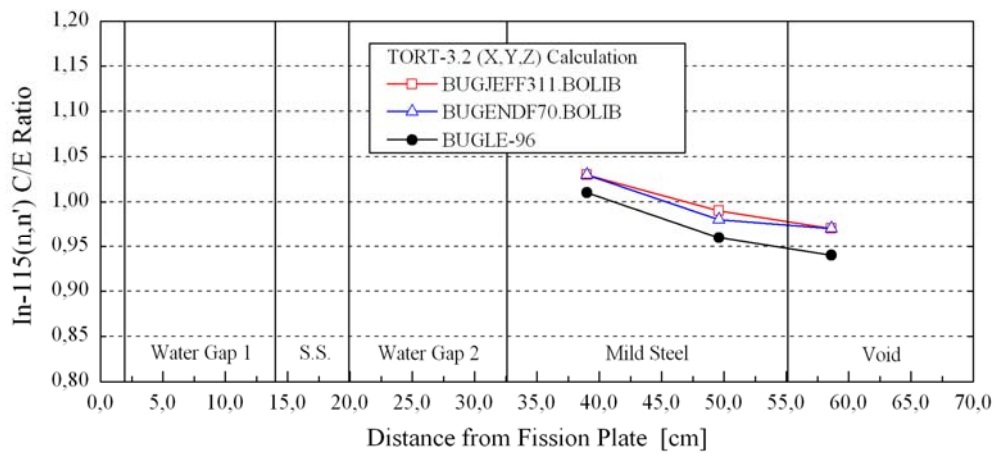


Figure 4. PCA-Replica - In-115(n,n') reaction rate ratios (Calculated/Experimental).

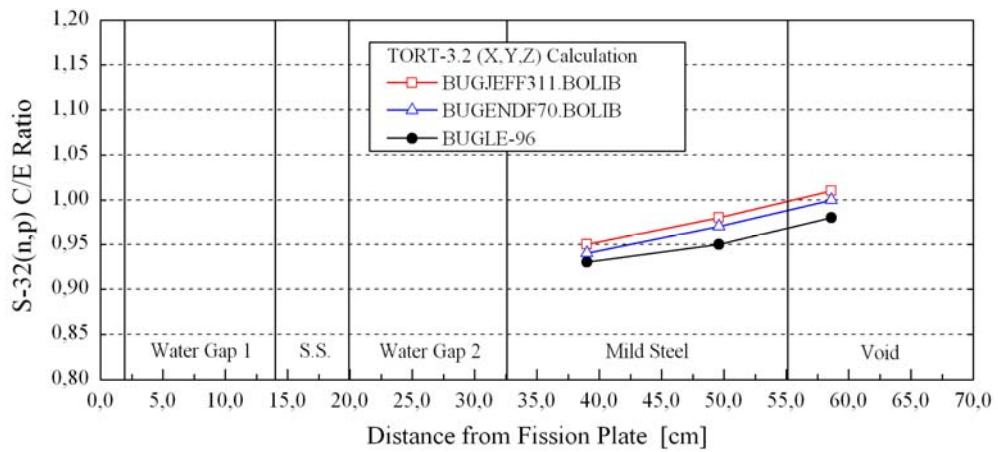
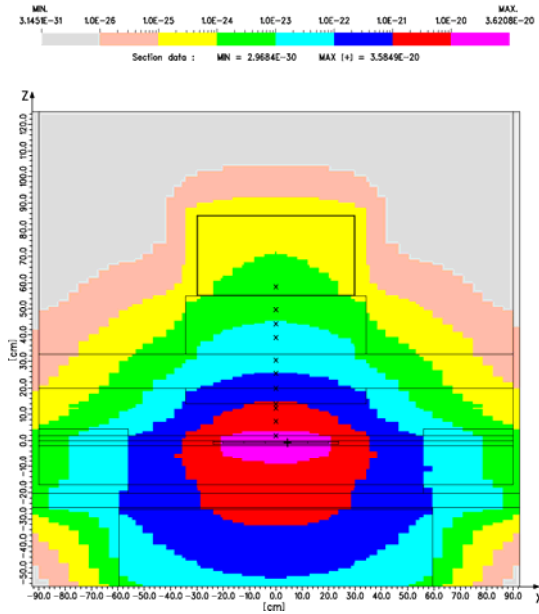
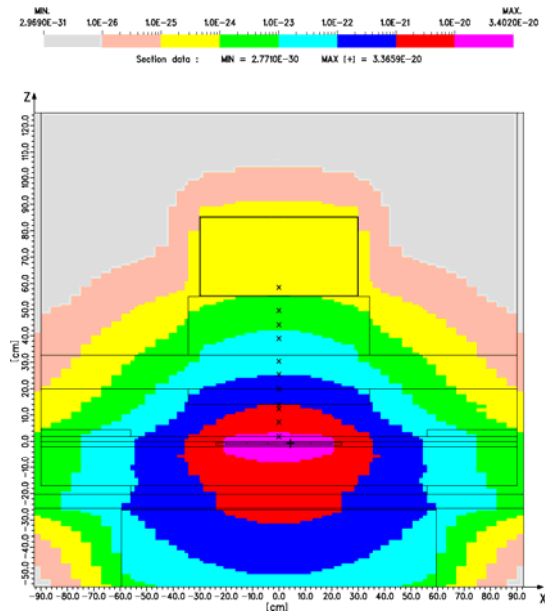


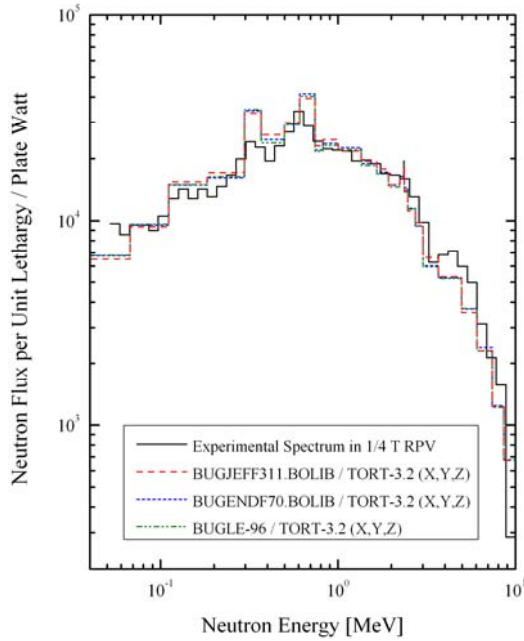
Figure 5. PCA-Replica - S-32(n,p) reaction rate ratios (Calculated/Experimental).



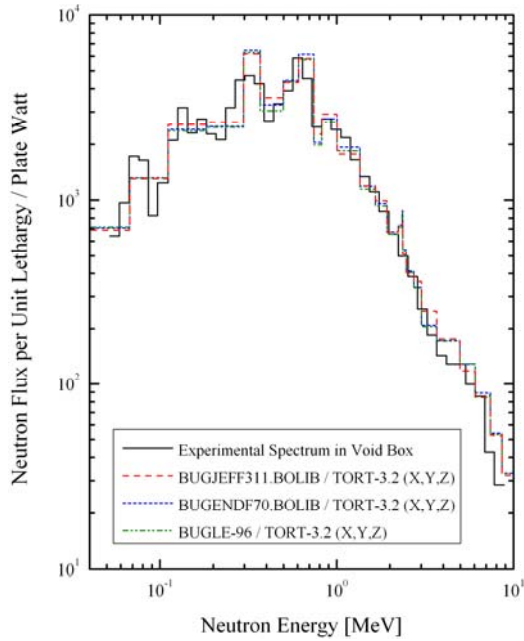
**Figure 6.** PCA-Replica - Spatial distribution of the Rh-103(n,n') reaction rates per NESTOR Watt. Horizontal section at Y = 0. cm, dosimeter locations "x", TORT-3.2 (X,Y,Z) with 65X×63Y×182Z spatial meshes. [reactions × s<sup>-1</sup> × atom<sup>-1</sup> × NESTOR Watt<sup>-1</sup>]



**Figure 7.** PCA-Replica - Spatial distribution of the neutron fluxes per NESTOR Watt for E > 1.0 MeV. Horizontal section at Y = 0. cm, dosimeter locations "x", TORT-3.2 (X,Y,Z) with 65X×63Y×182Z spatial meshes. [neutrons × barn<sup>-1</sup> × s<sup>-1</sup> × NESTOR Watt<sup>-1</sup>]



**Figure 8.** 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 9.** PCA-Replica - Comparison of experimental and calculated neutron spectra in air, in the void box measurement position at Z = 58.61 cm.



The calculated results obtained using BUGJEFF311.BOLIB and BUGENDF70.BOLIB appear in general to be almost always slightly higher with respect to the corresponding BUGLE-96 results. The use of the 1/4 T RPV weighting neutron dosimeter cross sections did not give meaningful differences in the steel measurement positions with respect to the corresponding calculated results obtained with the flat weighting cross sections. Adopting the same normalization per NESTOR Watt indicated in Table 1, the spatial distributions of the Rh-103(n,n') reaction rates and of the neutron fluxes with neutron energies above 1.0 MeV are shown in the same horizontal section at  $Y = 0$ . cm in Figures 6 and 7 respectively. The use of a fission neutron source with homogeneous spatial distribution implies a systematic slight (few percents) underestimation in the C/E dosimeter results with respect to the corresponding ones obtained with the inhomogeneous spatial distribution. The analysis of the dosimetric results got from calculations with several combination of  $P_N$ - $S_N$  approximations was limited to two key measurement positions: 1/4 T RPV (mild steel) and void box (air). In the  $P_3$ - $S_8$  calculations, slight C/E differences (few percents higher) for all the dosimeters were found in both measurement positions with respect to the corresponding C/E values obtained from the  $P_3$ - $S_{12}$  and  $P_3$ - $S_{16}$  calculations which, on the contrary, gave C/E results fully stabilized for all the dosimeters. In the  $P_5$  calculations, all the C/E results appear completely stabilized for all the dosimeters in both measurement positions, i.e. no meaningful C/E difference for a given dosimeter is evident between the corresponding results of the  $P_5$ - $S_{12}$  and  $P_5$ - $S_{16}$  calculations.

The neutron spectra calculated in the 1/4 T RPV and in the void box measurement positions using BUGJEFF311.BOLIB, BUGENDF70.BOLIB and BUGLE-96 are compared with the corresponding experimental neutron spectrum and are respectively shown in Figures 8 and 9. The normalization per fission plate Watt is assumed in the previously cited figures as in reference [1]. The group values of the experimental neutron spectra were taken from the corresponding “as measured” data reported in reference [1] and were reduced by 4% to eliminate the contribution from the NESTOR core neutron leakage background in the RPV and void box.

## 4 Conclusion

The ENEA-Bologna libraries BUGJEFF311.BOLIB and BUGENDF70.BOLIB permitted to obtain dosimetric and spectral results for the PCA-Replica shielding benchmark experiment comparable with those produced by the ORNL BUGLE-96 library. The deviations of the dosimetric results from the corresponding experimental ones are within the desired  $\pm 10$ -15% target accuracy. Given that the total experimental uncertainty ranges up to approximately 5% ( $1\sigma$ ), then the computational results presented in this paper exhibit very good statistical consistency with the corresponding measurements.

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