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JPDR Activation Analysis Benchmark
Using VITAMIN-B6 and BUGLE-96 Data**

John R. White

**Chemical and Nuclear Engineering Department
University of Massachusetts-Lowell, Lowell, MA 01854**

**Radiation Protection & Shielding Topical Meeting
Nashville, Tennessee
April 19-23, 1998**

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John R. White
University of Massachusetts Lowell
Lowell, Massachusetts 01854
Email: john_white@uml.edu

Abstract

This paper summarizes the latest UMass-Lowell JPDR benchmark results. Its primary goal is to present a verification benchmark for the DORT-ACTIV sequence for performing neutron activation calculations using the VITAMIN-B6 and BUGLE-96 data libraries. A comparison of the computed and measured activities for several isotopes included as part of the JPDR experimental program shows good agreement for most data points up to and including the reactor vessel, with a variability of about $\pm 30\%$. A few anomalous points with high computed values were observed for the ^{54}Mn activity. The high energy threshold reaction in ^{54}Fe that produces ^{54}Mn makes this activity very sensitive to data uncertainties and modeling approximations. The JPDR bioshield data were not included in the present verification because of the large modeling and geometry uncertainties that exist. The current benchmark exercise successfully validates the general computational procedure and data libraries used in the present analyses, but additional studies are still needed for confirmation that the DORT-ACTIV sequence can adequately predict individual isotope activities well into the bioshield region.

Introduction

The University of Massachusetts Lowell (UMass-Lowell) took part in an international benchmark exercise organized by the IAEA to address the adequacy of current cross section data and computational methods for quantifying neutron activation in the excore regions of commercial power reactors.¹ The main focus of the benchmark exercise involved the comparison of calculated results to measured activation data from the Japan Power Demonstration Reactor (JPDR).²⁻³ The available experimental data include radial and axial activity profiles at various locations in the excore structure and bioshield regions for several important radioactive isotopes. The unique aspect of the UMass-Lowell work was the use of the ACTIV code⁴ - a recently-developed space-energy activation analysis capability that takes full advantage of the detailed multigroup information available from a transport theory calculation of the neutron flux distribution in the excore regions of power reactors.

The original UMass-Lowell benchmark calculations were completed in 1995 and summary results from that work are given in Ref. 4. The original calculations were based on a 47-group activation analysis library that was derived from a pre-release version of the VITAMIN-B6 library (early 1994 vintage). The transport calculations were done with the BUGLE-93 shielding library. In late 1996 an official release of an updated VITAMIN-B6 library was made available through the Radiation Shielding Information Computational Center. In addition, the BUGLE shielding library was updated and corrected (there was an error in BUGLE-93 in the weighting function used to collapse the neutron cross sections) and released as BUGLE-96. On the local level, some minor errors were also found in the original JPDR RZ DORT models used to generate the results in Ref. 4. With all the uncertainty associated with modeling errors, cross section processing errors, and with the impact of an updated base library, it was decided that a complete reanalysis of the JPDR benchmark was needed.

This paper briefly overviews the data and methods used to generate the latest JPDR benchmark results and it gives a comparison of the computed and measured activities for several isotopes included as part of the JPDR experimental program. Previous works have consistently identified that the insufficient geometric and material composition information for the JPDR bioshield leads to poor agreement with measured data in this region.⁴⁻⁶ Since no new bioshield information is available, the current results emphasize the capability of a DORT-ACTIV sequence to predict long term neutron activation in the excore components up to and including the pressure vessel region. Some data for the surface and interior of the bioshield are included for future reference, but these data are not considered as part of the DORT-ACTIV verification effort at this time.

Data and Methods

The current UMass-Lowell JPDR benchmark computations used the DORT code and the BUGLE-96 library for all the 2-D RZ JPDR transport calculations. The BUGLE-96 broad-group dataset was collapsed from the ENDF/B-VI VITAMIN-B6 fine-group library with a specific focus on shielding applications. This library is readily available to the user community and it is routinely used for excore radiation transport computations.

The new ACTIV code was used for the activation calculations.⁴ This code eliminates much of the uncertainty associated with the use of few-group ‘effective’ activation cross sections by performing the activation calculations with the same space and energy dependent detail that was used in the transport theory computation for the neutron flux distribution. The same geometry is modeled and the user can select any number of pointwise radial and axial traverses or zone average activations, as desired. Thus, all of the space-energy detail from the original transport computation is preserved and included within the activation calculation.

For full consistency, the activation cross sections used within ACTIV were also derived from VITAMIN-B6. A new ACTXS47.LIB 47-group activation library was generated using several modules of the SCALE 4.3 system, an updated version of ACTXS (a cross section processing code written specifically for generating data for ACTIV),⁴ and a concrete weighting function consistent with that used to develop the BUGLE-96 package. Data for eight reaction types (n,γ , n,α , n,p , $n,2n$, n,d , n,t , n,f , and total neutron absorption) were extracted from the collapsed library and stored in a format suitable for use in ACTIV. This new activation library is intended for use with a DORT-ACTIV analysis sequence, with the DORT transport calculation based on BUGLE-96 cross sections. The BUGLE-96/DORT calculation determines the appropriate multigroup fluxes and the ACTXS47.LIB/ACTIV computation determines the space and time dependent activities for the desired excore locations.

The remaining data needed for the activation calculations (natural isotopic abundances, decay data, and appropriate branching fractions) were obtained from the ENDF/B-VI version of the ORIGEN data libraries that are distributed as part of the SCALE 4.3 package. The necessary data were extracted from the ORIGEN data files and incorporated into the activation library used within ACTIV.

The ACTIV code itself uses the traditional matrix exponential technique for solution of the nuclide transmutation equations. The ACTIV code simply reads the appropriate nuclide chain information, geometry data, initial isotope densities, and operational power versus time data and, using the precomputed space-energy fluxes from DORT (or some other transport analysis code) and the nuclear data from the activation library, computes the time-dependent isotope inventories for each spatial point or zone of interest. The summary edit from ACTIV gives the activity in Bq/g or Ci/g for the desired isotopes, spatial locations, and time points. These data can then be plotted or tabulated for further analyses.

JPDR Modeling within DORT

The Japan Power Demonstration Reactor (JPDR) was a direct-cycle BWR with dimensions that spanned over 12 m axially and 4 m radially. The reactor operated intermittently with varying power level over a period of about 13 years, from 1963 to 1976, with a total reactor thermal output of 21,500 MWD. As outlined in Ref. 4, the 12.2 m axial dimension was broken into three regions and labeled accordingly, with Region 1 at the bottom and Region 3 at the top. A bootstrapping technique, which couples one axial region to another via a saved internal boundary source is envisioned as a mechanism to complete the full benchmark computation. Modeling of the JPDR started at Region 2 which contains the core, and hence, the neutron source which drives the entire model. At present, the Region 2 model is the only computation that has been completed and fully analyzed.

An overall radial dimension of 300 cm was used in the DORT models. Reflected boundary conditions were employed on the left and right model boundaries, and vacuum conditions were imposed on the top and bottom of the Region 2 RZ model. The final JPDR DORT model has a concrete bioshield containing explicit zones that account for several cooling tubes and structural rebar reinforcements. This model, with an overall 155 x 201 mesh grid, represents an improvement over the initial JPDR configuration documented in Ref. 2 with additional bioshield data from Ref. 3. However, the modeling information for the bioshield portion of the overall configuration is still not sufficient for a detailed verification test of the methods and data. Thus, in the present work, not much emphasis is placed on this region of the JPDR model.

The final model here also differs slightly from the one discussed in Ref. 4 in that a finer mesh structure is used in the current model (the Ref. 4 results were based on a computational model with 118×123 mesh points) and a single symmetric S_{16} quadrature set is used for the angular discretization (a variable quadrature scheme within DORT was adopted previously). The present model, referred to as Case D, includes the axial region from 90 cm to 509 cm above the bottom of the JPDR reactor vessel.

The material compositions used in the final Case D Region 2 JPDR computational model were taken directly from Ref. 2, except for the more explicit modeling in the bioshield region (the bioshield data were derived from Ref. 3). The space-energy source distribution within the core region of the JPDR model was also obtained from information given in Ref. 2. The total source was normalized such that 1 MW of thermal power is generated within the core. The actual power level at any specific time is handled within ACTIV via a simple time-dependent normalization of the absolute flux for the 1 MW power case. P_3 scattering data were used in all the calculations.

Some DORT Results for the JPDR Region 2 Model

DORT calculations were made with the model described above and the multigroup scalar fluxes were saved for use in ACTIV. In addition, collapsing of the fluxes to three broad groups was performed for summary presentation of key radial and axial flux profiles. Several multigroup activity cross sections were also collapsed to the three-group level and to a single effective broad group for summary review of the spatial dependence of these 'effective' cross sections versus position within the system. Of particular interest were the few-group flux and cross section profiles in the locations where measured activity data are available. The microscopic reaction rate profiles (reactions per second per target atom) for several key reactions were also generated from these few-group data. These data can provide considerable insight into the activation analysis problem.

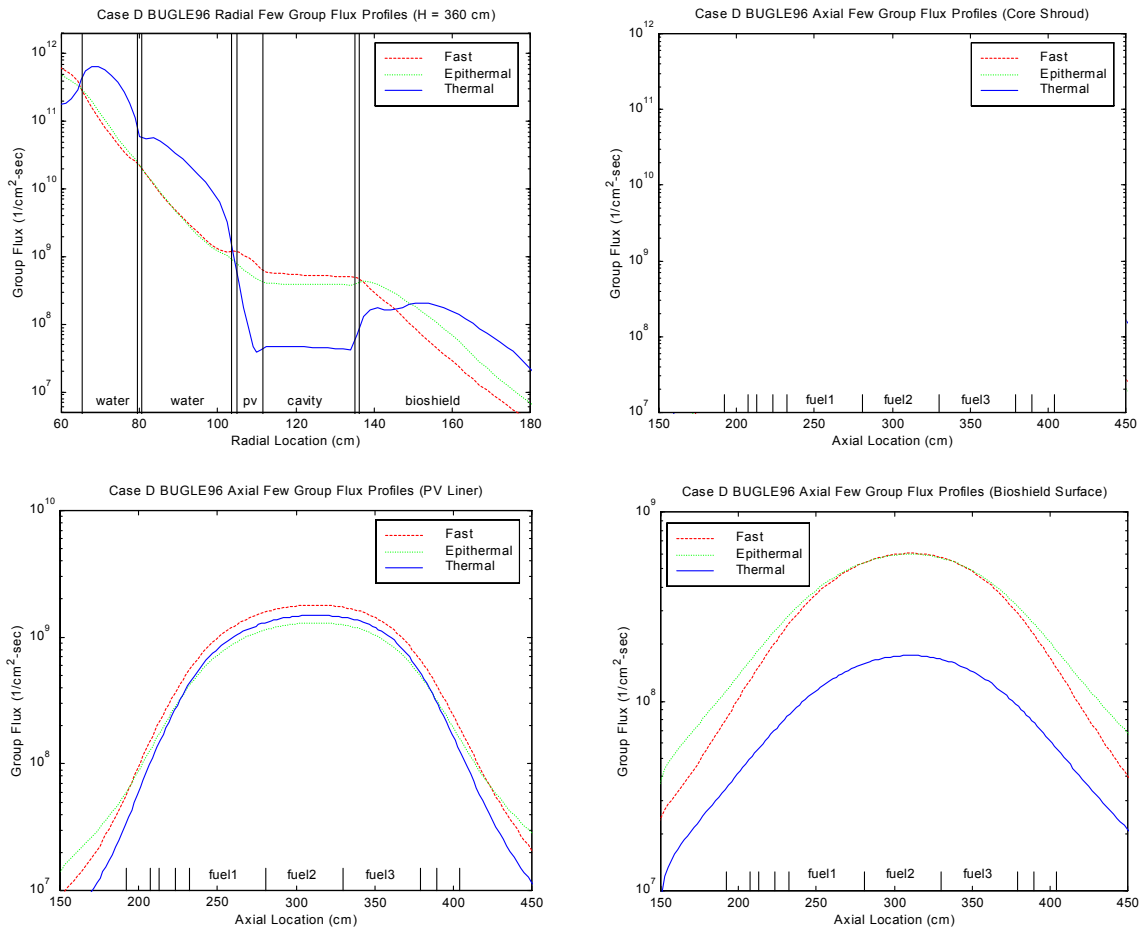


Fig. 1. Selected broad-group radial and axial flux profiles from the JPDR Case D model.

The unique aspect of the ACTIV code is its ability to easily incorporate the full space-energy coupling that is inherent in real systems. The transport theory computations produce all the needed neutron distribution information, but this detail is often ignored or used in an approximate fashion in most analyses. With the availability of a fully compatible multigroup activation library, it becomes a relatively simple process to utilize all the available space-energy detail to eliminate much of the uncertainty that is often associated with most zero-dimensional activation analysis studies. As an illustration of some of the information that is lost (or approximated) in zero-dimensional studies, the remainder of this section is devoted to displaying some subtle, but often important, space-energy coupling phenomena that occur in the excore regions of LWR systems.

As indicated above, the 47-group data from the actual calculations were collapsed to three broad groups for presentation purposes. The spatially dependent data focus on the radial distributions in the reactor's pressure vessel (PV) and the concrete biological shield (bioshield) at a height of 360 cm above the bottom of the reactor vessel, and on the axial profiles at the core shroud, PV liner, and bioshield surface. Measured activity data for several isotopes are available from the JPDR experimental program at these locations. Flux, cross section, and reaction rate profiles are highlighted in the following discussion.

In particular, Fig. 1 shows several typical radial and axial broad-group flux profiles obtained from the JPDR computational model. Group 1 represents fast neutrons above 0.1 MeV, Group 3 is the thermal group with energies below 0.4 eV, and Group 2 covers all energies between these limits. Although the profiles behave qualitatively as expected, they also illustrate, quite clearly, the rapid changes in neutron spectra that occur at various locations throughout the excore regions. For example, the radial plot clearly shows the attenuation of thermal neutrons in the thick vessel structure and the thermalization of the hard spectrum on the surface of the bioshield with only about 10-20 cm penetration into the shield region. Similar effects can be seen in the axial

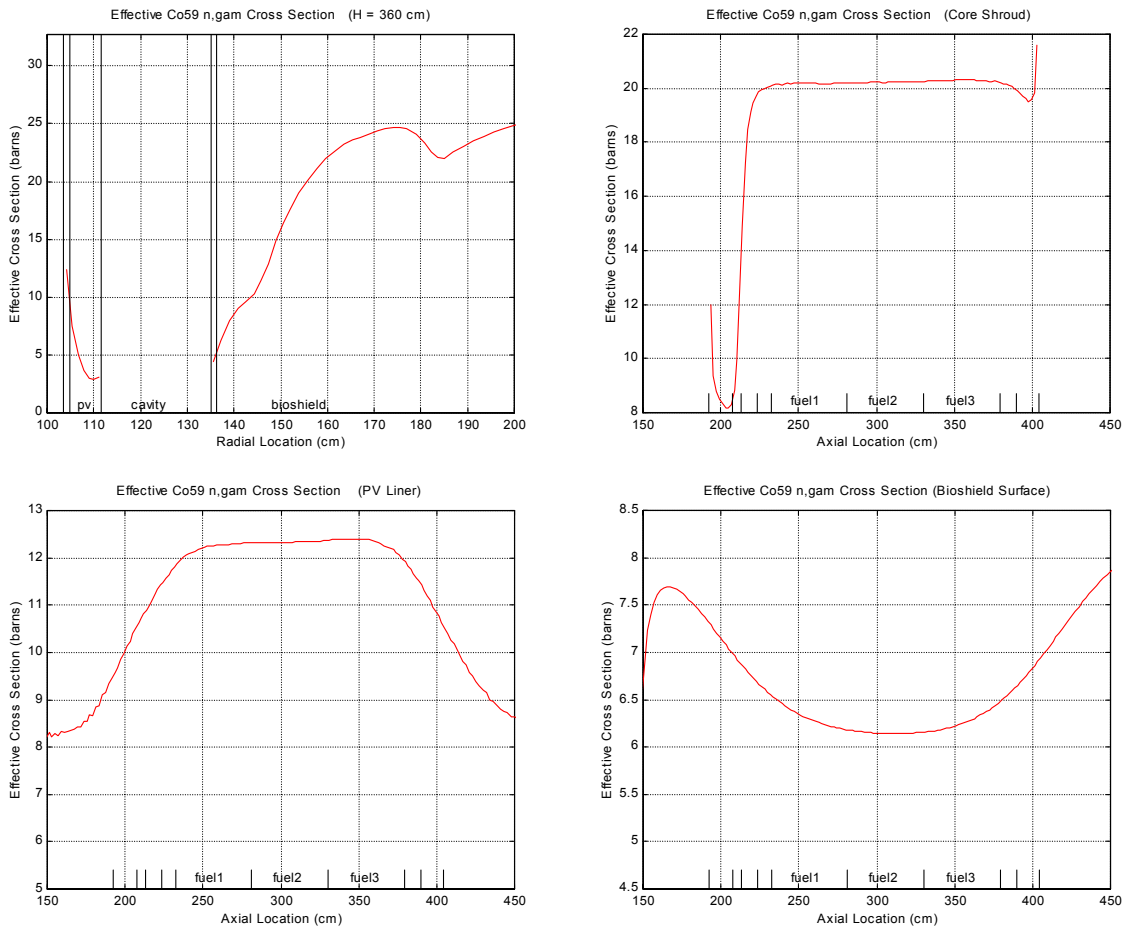


Fig. 2. Selected ^{59}Co n,gam effective cross section profiles from the JPDR Case D model.

profiles as one moves farther from the core region. Although spectral changes in the axial direction at any given radial location are relatively small, the changes observed when moving radially outward from the shroud, to the vessel surface, to the surface of the bioshield are indeed significant.

The impact of these spectral shifts can be illustrated by computing the effective activation cross sections versus position, taking into account the explicit change in the multigroup weight function at each spatial point. A typical example is given in Fig. 2 which shows the effective 1-group ^{59}Co n, γ activation cross section versus position corresponding to the flux profiles given in Fig. 1. The key observation here is the large variation in the effective cross section versus position. In particular, the 1-group average cross section for ^{59}Co varies by about a factor of 4-5 in the two radial regions shown in Fig. 2 and by a factor of two or more in specific axial regions. This type of variability is typical and it simply indicates that large spectral shifts do occur. This phenomenon is certainly significant and it must be treated with care if reliable activation calculations are desired. Since the ACTIV code models this space-energy coupling in full detail, all the uncertainty related to the use of zone and energy averaged cross sections in the usual zero-dimensional activation analyses is eliminated completely.

The variation in the effective 1-group cross sections is an indication of changing neutron spectra. The quantity actually used in the activation calculations is the micro reaction rate with units of reactions/sec per atom. This parameter is just the reaction cross section times the flux integrated over energy. The spatial variation of the ^{59}Co n, γ reaction rate per atom for the same locations as above is illustrated in Fig. 3. These data include both spectral variations and the spatial attenuation of the total neutron flux. The spectral component of the reaction rate information can be isolated by plotting the fractional contribution of each energy group to the total reaction rate. This has been done for the ^{59}Co n, γ reaction rates in Fig. 4, which clearly shows a considerable epithermal contribution in portions of many components.

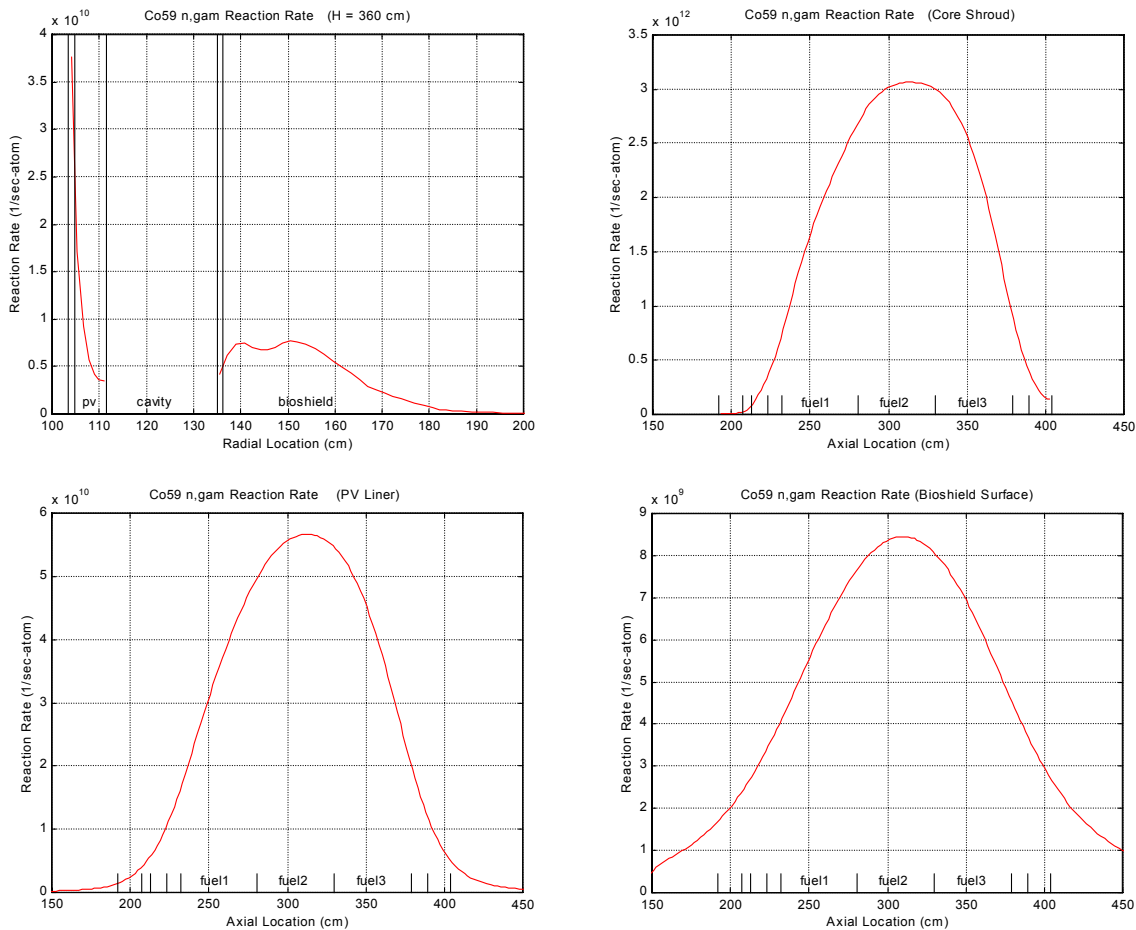


Fig. 3. Selected ^{59}Co n, γ reaction rate profiles (reactions/sec per atom) for the Case D model.

There is a significant amount of information contained in Figs. 1-4. These details are not generally available and they are not absolutely essential to the user. However, with this information, a lot of insight into the physics of the activation calculation can be obtained, especially relative to the importance of space and energy coupling in typical LWR systems. However, what is critically important is that these effects be properly treated within the activation computation. If care is taken by the user, these phenomena can be approximately incorporated manually within zero dimensional codes. The ACTIV code, on the other hand, automatically does this without specific interaction from the user. All important effects are treated from basic physics principles.

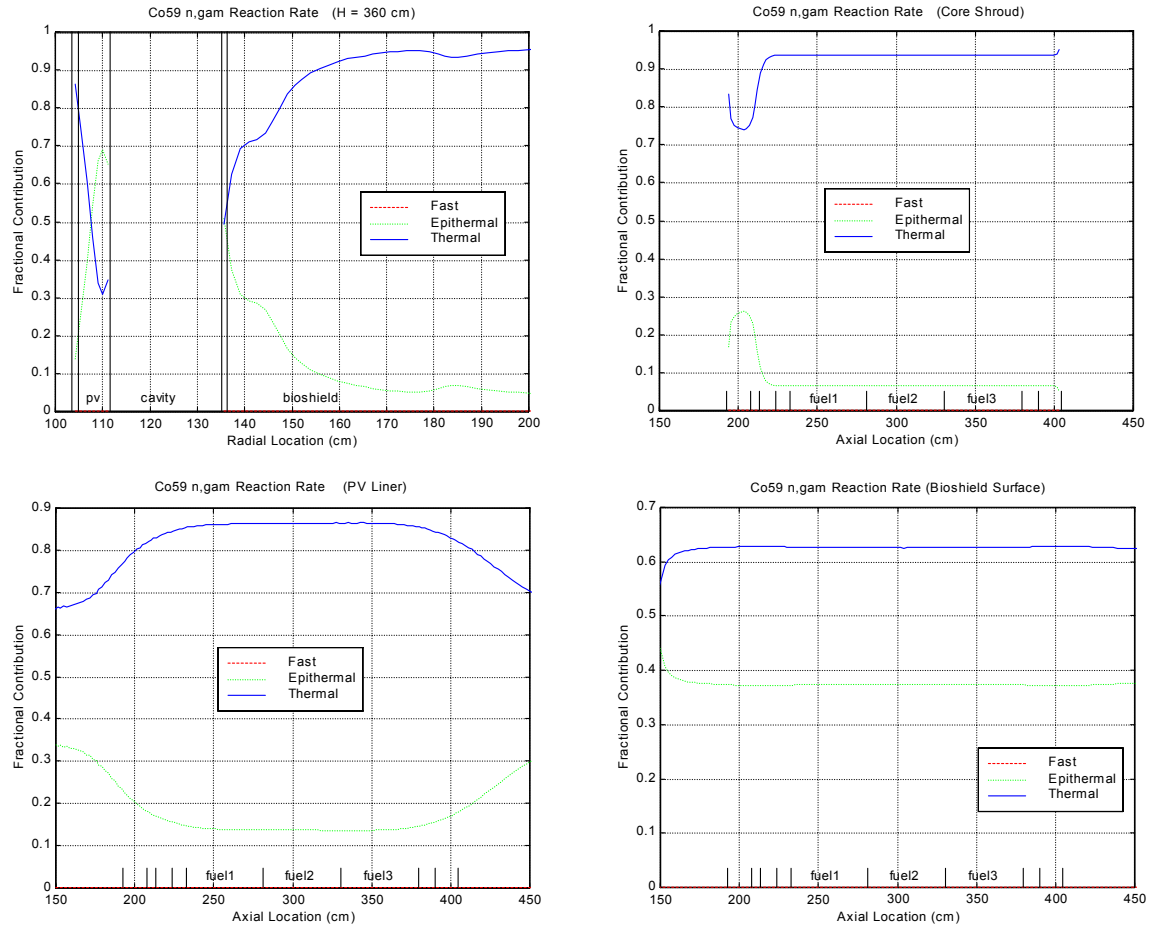


Fig. 4. Fractional contribution by broad group for the ^{59}Co n, γ reaction rate profiles.

Activation Analysis Results

ACTIV was run using the 47-group fluxes from the DORT run and the primary production routes and decay data associated with ^{54}Mn , ^{55}Fe , ^{60}Co , ^{63}Ni , ^{152}Eu , and ^{154}Eu . The current calculations focused only on these activation products because these were measured as part of the experimental program in the JPDR. The initial parent densities associated with these daughter products were obtained from Ref. 2.

The summary results from ACTIV highlight several radial and axial activity profiles. The radial profiles focus exclusively on the ^{60}Co activity, first in the pressure vessel and then in the bioshield. These data are plotted in Figs. 5 and 6. Each figure has two components. The first part shows a plot of the absolute activities, with the circles representing the measured values and the solid line giving the computed values. The second figure in each set displays the behavior of the ratio of the calculated-to-experimental value (C/E value) with the asterisks showing the actual C/E value at each measurement location and the solid line representing a low-order best fit to these individual points. For the pressure vessel, a quadratic fit was used and, in the bioshield, a simple linear fit was used for the C/E profile. The fits are used to simply show the general trend in the C/E data.

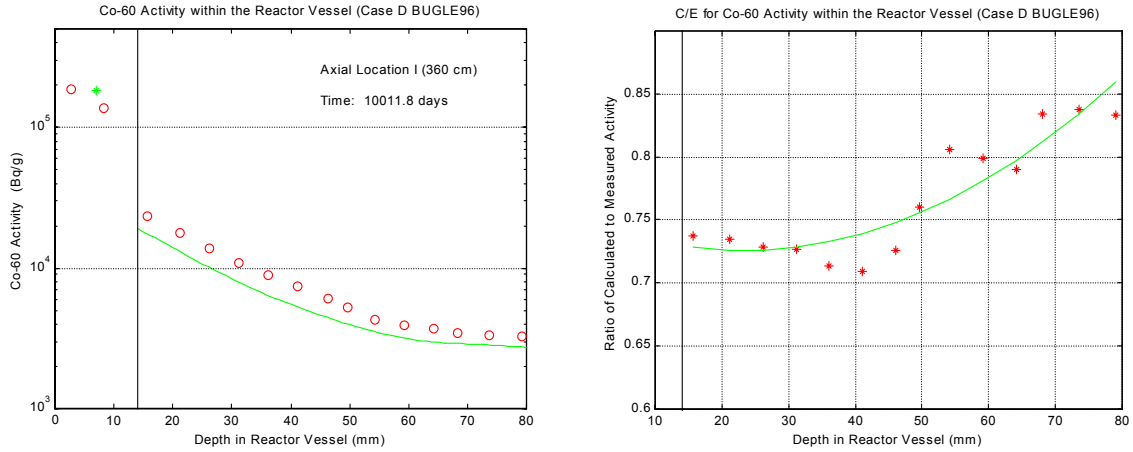


Fig. 5. Radial activity and C/E profiles for ⁶⁰Co within the reactor vessel.

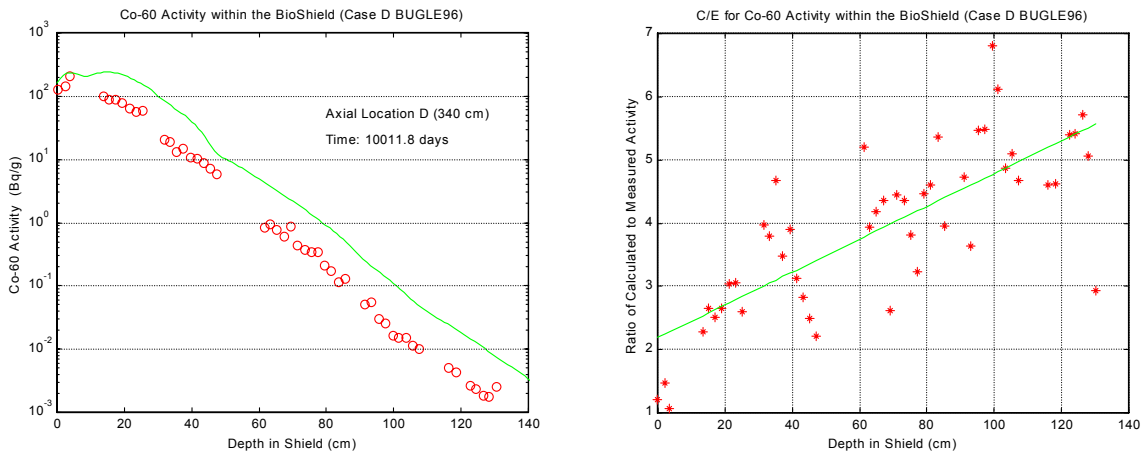


Fig. 6. Radial activity and C/E profiles for ⁶⁰Co within the bioshield.

The axial activity data for the core shroud and PV liner are summarized in Table 1. The C/E values for four radioactive isotopes are given at the specific measurement locations. There are only three measured values in the shroud and five experimental points in the PV liner over the axial range treated in these computations.

Discussion of the Results

Concerning the plots and tabular data, one can argue that generally good results were obtained for most radial and axial points through the pressure vessel region of the JPDR model. For example, the C/E values in Fig. 5 show that the radial distribution of the ⁶⁰Co activity is under-predicted by 15% to 30% (C/E range is from 0.85 to 0.70). Most of the axial profile C/E values in Table 1 also show good agreement with experiment to within $\pm 30\%$.

The only exception to the above statement is associated with the ⁵⁴Mn activity at the lowest measured point in both the shroud and PV liner. In both cases, the DORT-ACTIV computations significantly over-predict the ⁵⁴Mn activity. This discrepancy is of concern, and no single good explanation for the large error is available. However, it should be emphasized that the absolute ⁵⁴Mn activity is very low relative to the other measured activities, that the ⁵⁴Fe n,p parent reaction has a high energy threshold, and that only the lowest measurement point, which is in the vicinity of the axial plane associated with the lower grid and support plate, has this problem. Clearly the modeling and homogenization approximations needed in this area could be the culprit. Also of note is the fact that no uncertainty information is available for any of the measured data or material concentrations given in Ref. 2. Thus, with all these considerations, it is important not to place too much significance in the poor agreement for these two data points - but they should not be simply ignored either.

Table 1. C/E values at several axial points along the core shroud and PV liner.

| | Core Shroud | | | PV Liner | | | | |
|------------------|-------------|---------|---------|----------|---------|---------|---------|---------|
| | Point 1 | Point 2 | Point 3 | Point 1 | Point 2 | Point 3 | Point 4 | Point 5 |
| ⁵⁴ Mn | 1.51 | 0.85 | 0.99 | 1.91 | 1.09 | 1.29 | 1.18 | 1.31 |
| ⁵⁵ Fe | 1.10 | 0.79 | 1.20 | 1.16 | 0.74 | 0.88 | 0.86 | 0.90 |
| ⁶⁰ Co | 1.03 | 0.93 | 1.11 | 1.13 | 0.70 | 0.83 | 0.81 | 0.84 |
| ⁶³ Ni | 1.18 | 1.01 | 1.03 | 1.07 | 0.69 | 0.82 | 0.80 | 0.84 |
| z loc (cm) | 240 | 305 | 376 | 206 | 256 | 306 | 328 | 368 |

Thus, except for a few anomalies, the general accuracy of the calculations, up to and including the vessel, is on the order of $\pm 30\%$. This is considered quite acceptable, especially considering the complexity and the many inherent uncertainties in the calculations. For example, although not explicitly stated, it is expected that the experimental data and the initial isotopic concentrations in the structural materials have combined uncertainties approaching the range of C/E values observed here.

However, the good agreement that was observed through the vessel was not achieved in the bioshield region. Good results were obtained at the bioshield surface, but the calculations significantly over-predict the measured activity at all points in the bioshield, and the error tends to grow with distance into the shield. This general behavior is consistent for all the bioshield isotopes. This poor agreement is attributed to the relatively cursory modeling information available for this portion of the JPDR. Although Ref. 3 improved upon the bioshield data from Ref. 2, there still is too much uncertainty in the precise geometry, concrete water content, measurement locations, etc., to allow adequate comparisons and conclusions to be drawn. This observation is consistent with other researchers.⁵⁻⁶ The conclusion, therefore, is simply that there is too much uncertainty in the JPDR bioshield geometry and operational data for it to be useful in the current benchmark. Further information from the JPDR experimental program or from some other source is needed for additional testing in the bioshield region.

Overall, the current benchmark validates the computational procedure and data libraries used here. There are several areas that could use further study (bioshield region, ⁵⁴Mn activity, other isotope activities, additional data comparisons in axial regions farther from the core, etc.), but the base methodology has been established as adequate for predicting excore activities after long-term exposure to a neutron field. The DORT-ACTIV combination is easy to use and it treats the basic physics of neutron activation with full space energy coupling. It represents one of the most comprehensive tools for performing analyses of this type. The JPDR benchmark computations performed here successfully demonstrate the utility of this approach to activation analysis.

References

1. N. Kocherov, "Benchmark on Radioactive Inventory Calculations for Fission Reactor Decommissioning," letter from IAEA to potential participants in benchmark exercise (1994).
2. T. Sukegawa, et. al., "Accuracy Verification for Calculation of Inventory in JPDR Due to Neutron Activation," International Atomic Energy Agency, INDC(JPN)-164 (1993).
3. Letter from N. Kocherov (IAEA) to J. R. White (UMass-Lowell) dated March 31, 1995 containing detailed drawings from JAERI describing the central part of the JPDR bioshield.
4. J. R. White and A. P. Fyfe, "UMass-Lowell Results for the JPDR Activation Analysis Benchmark," 1996 Topical Meeting on Radiation Protection and Shielding, No. Falmouth, Massachusetts (April 1996).
5. B. L. Broadhead and R. L. Childs, "ORNL Contribution to the IAEA Benchmark Problem on Fission Reactor Decommissioning," 1996 Topical Meeting on Radiation Protection and Shielding, No. Falmouth, Massachusetts (April 1996).
6. S. J. Wall, et. al., "Current Status of UK Calculations for IAEA Decommissioning Benchmark (JPDR)," 1996 Topical Meeting on Radiation Protection and Shielding, No. Falmouth, Massachusetts (April 1996).