UMass-Lowell Results for the JPDR Activation Analysis Benchmark

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ABSTRACT

An international benchmark activity that focused on the data and methods available for performing neutron activation analysis in reactor structural and shielding materials has recently been completed. The benchmark includes comparisons with measured data from the Japan Power Demonstration Reactor. This paper describes the data and methods utilized and the results obtained as part of the University of Massachusetts Lowell contribution to this computational benchmark activity. Also highlighted is the use of a new fully-coupled space-energy activation analysis code called ACTIV.

I. INTRODUCTION

The University of Massachusetts Lowell (UMass-Lowell) was an active participant in an international benchmark exercise organized by the International Atomic Energy Agency (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 central 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 (^{60}Co, ^{54}Mn, ^{55}Fe, etc.). The unique aspect of the UMass-Lowell work was the use of a newly-developed space-energy activation analysis code called ACTIV. The purpose of this paper is to document the UMass-Lowell results for the JPDR activation analysis benchmark and to highlight the new capabilities within ACTIV.

II. DATA, METHODS, AND CODES

The nuclear data needed for neutron activation studies fall into two categories:

1. multigroup neutron cross sections for use in the transport calculations to compute the space and energy dependence of the neutron flux, and
2. multigroup activation cross sections and decay data for all the important parent and daughter isotopes that can be generated via neutron activation.

If possible, the transport calculation and the activation analysis should be done with a consistent set of multigroup data. However, in practice, the two calculations are often done independently and are only loosely connected via a set of collapsed neutron flux information from the transport

calculation that is used in zero-dimensional few-group codes that model and simulate the isotope transmutation schemes. Usually significant detail is lost in this space and energy collapsing process, which can lead to large uncertainties in the computed activities. This is especially true in regions where rapid changes in the neutron spectra cannot be treated adequately in a zero-dimensional model. In addition, the coupling process is often somewhat cumbersome, since it usually requires a fair amount of manual intervention and data transfer among several codes.

The new ACTIV code eliminates this separate coupling and collapsing process by performing the activation calculations with the full space and energy dependent fluxes from the transport code. 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 – thereby, removing all the additional uncertainty that is introduced in the traditional two-step process.

The UMass-Lowell benchmark analysis used the DORT code[4] and the BUGLE-93 library[5] for all the 2-D JPDR transport calculations. The BUGLE-93 broad-group dataset was collapsed from the VITAMIN-B6 fine-group library[5] with a specific focus on shielding applications, and it is not usually considered as a database for determining thermal fluxes and reaction rates – since there are only two energy groups below 0.4 eV. However, it does have several positive attributes including the fact that it contains the latest ENDF/B-VI data, it is readily available to the user community, and it already has a wide user base. Thus, it was decided that BUGLE-93 would be used exclusively for the 2-D DORT computations.

For full consistency, the activation cross sections used within ACTIV were also derived from VITAMIN-B6. The VITAMIN-B6 199-group neutron data were collapsed to the BUGLE-93 47-group structure using the same concrete weighting spectrum utilized in the generation of BUGLE-93 from VITAMIN-B6. 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.

In addition to the neutron cross sections, natural isotopic abundances, decay data, and appropriate branching fractions are also needed for the activation calculations. These data were obtained from the ENDF/B-VI version of the ORIGEN data libraries that are distributed as part of the SCALE 4.2 package.[6] The necessary data were extracted from the ORIGEN data files and incorporated into the activation library used within ACTIV.

The final activation library, called ACTXS47.LIB, has all the required nuclear data for subsequent activation analyses within ACTIV. This library contains base information for approximately 800 isotopes (nuclides from the ORIGEN data files), but it only has activity cross sections for about 100 isotopes (nuclides from the VITAMIN-B6 library). However, as new cross section information for additional isotopes becomes available (in the VITAMIN-B6 master library format), it can be incorporated within ACTXS47.LIB quite easily.

A simplified schematic that illustrates the development of the activation library used within ACTIV is shown in Fig. 1. This figure summarizes the various steps involved in the generation of the specific 47 group library, ACTXS47.LIB, which is compatible with the BUGLE-93 library used in the transport

computations. If used with another dataset, only the energy grid and weight function would be modified. Most of the codes mentioned (MALOCS, NITAWL-II, ALPO, and ORIGEN) are part of the SCALE 4.2 package.[6] ACTXS, the last code in the sequence, was written as part of this work to integrate all the necessary nuclear data into a single file for use in ACTIV.

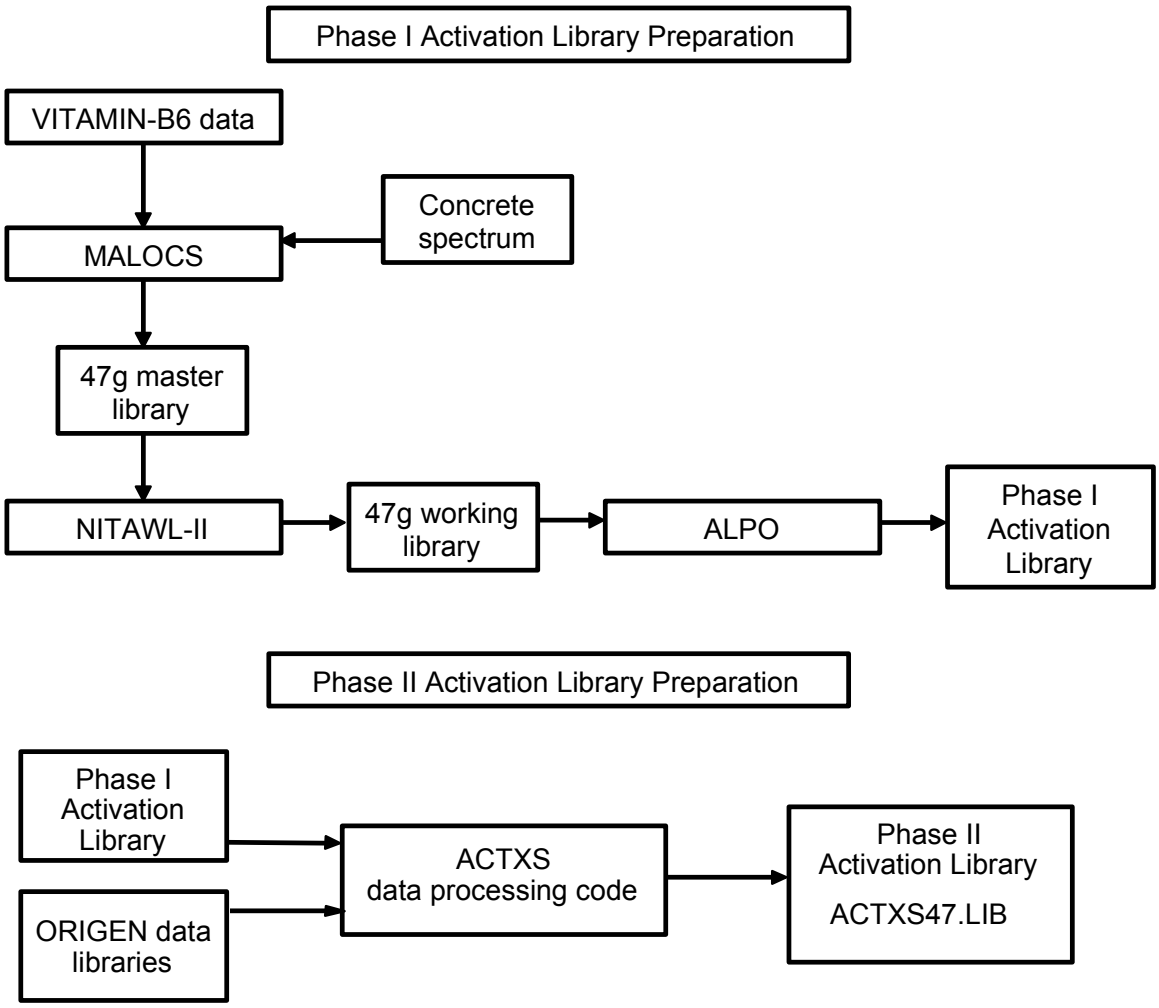

Fig. 1 Simplified schematic showing the development of the ACTXS47.LIB activation library.

The ACTIV code itself uses the traditional matrix exponential technique for solution of the nuclide transmutation equations. The primary computational algorithms for the matrix exponential method were taken from the DEPTH-CHARGE modules of the VENTURE code system.[7] 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 data flow and interaction between DORT and ACTIV are illustrated in Fig. 2. The summary edit from ACTIV gives the activity in Bq/g for the desired isotopes, spatial locations, and time points. These data can then be plotted or tabulated for further analyses – which, in the present JPDR benchmark study, involves direct comparison to the measured data from Ref. 2.

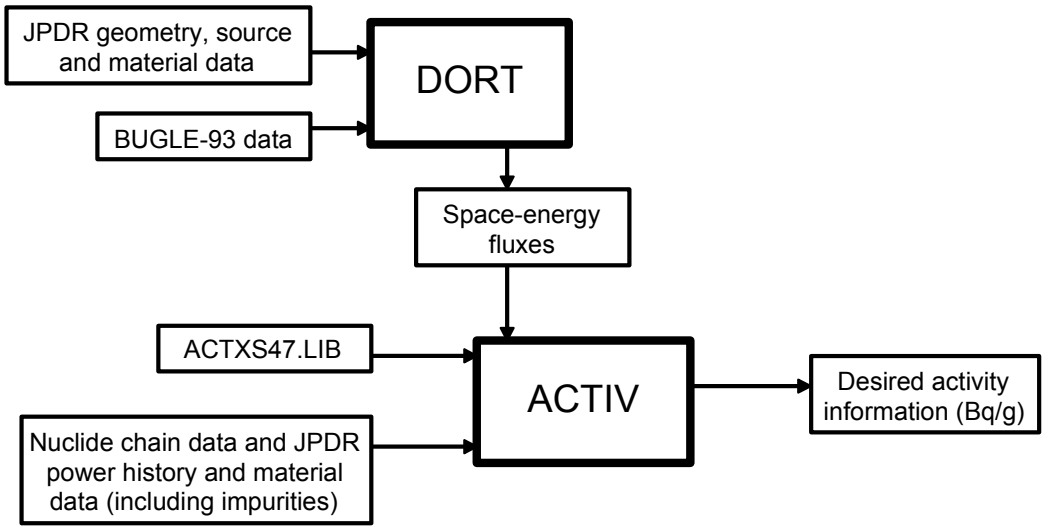

Fig. 2 Data flow and interaction between DORT and ACTIV.

III. JPDR MODELING WITHIN DORT

The bulk of the effort needed for performing the JPDR benchmark analyses was related to the development and execution of the DORT models that were used to compute the space-energy distribution of the flux throughout the system. 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.

It was apparent that the overall computational model would have to be broken into multiple sections axially, since a single DORT calculation with sufficient detail would be somewhat impractical. Therefore, 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.

An overall radial dimension of 300 cm was used in the DORT models, with the radial fine mesh layout remaining the same in each axial model so as to maintain spatial continuity from one axial region to the next. This continuity is required for proper alignment of the saved boundary sources that couple the axial models. The axial locations of the saved boundary sources are in relatively homogeneous regions well above and below the active core zones. These locations seem very reasonable, since they allow regions of practical size to be modeled while, at the same time, placing the boundary sources in regions relatively far away from structural materials where backscatter may be important.

Modeling of the JPDR started at Region 2 which contains the core, and hence, the neutron source which drives the entire model. This is the only computation that has been completed at present. However, internal sources were saved at an axial distance of about 100 cm from the top and bottom

boundaries of the model. These sources can be used to continue computations into the upper and lower structural regions of the JPDR configuration, if desired. 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 (with a 118 x 123 mesh grid). This model represents an improvement of the initial JPDR configuration documented in Ref. 2 with significantly more detailed bioshield data from Ref. 3.

The material composition data for the various zones within the final Region 2 RZ model were taken from Refs. 2 and 3. Although P_5 scattering is available within the BUGLE-93 library, only P_3 data were used in these benchmark calculations. Also, because of the size of the computational model, a variable quadrature scheme within DORT was adopted to help cut back on the overall computational time. An S_{16} symmetric quadrature was used in the more important regions and in the vicinity of the cavity, and an S_8 quadrature set was used in all remaining areas. Preliminary calculations with a single S_{16} quad-rature throughout the full model verified the validity of the variable quadrature approximation.

The final information necessary to run DORT was the space-energy source distribution within the core region of the JPDR model. Numerical estimates of the spatial source distribution were obtained from Figs. A.2 and A.3 in Ref. 2. A spline fit to the discrete radial and axial profiles produced a continuous distribution and, with this information, the relative source strength associated with the specific mesh spacing utilized in the UMass-Lowell JPDR models was obtained. The RZ spatial source distribution is then simply the product of the radial and axial profiles, $S(r,z) = S(r)*S(z)$.

The source energy spectrum for the 47-group computations was obtained by integrating the Watt fission spectrum over the appropriate 47-group energy grid. 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.

With all the necessary data defined, the DORT calculations were made with a pointwise convergence criterion of 0.001. The full space and energy dependent scalar flux data were saved for subsequent use in ACTIV. In addition, some post-processing of the multigroup data – collapsing of the data to three broad groups – was performed for summary presentation of key radial and axial flux profiles. Of particular interest were the profiles in the locations where measured activity data are available.

Figure 3 shows a typical radial broad-group flux profile 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. The radial profiles in Fig. 3 are for a height of 360 cm, which corresponds to the location where the measured horizontal distribution of the ^{60}Co activity within the pressure vessel is available. Although the profiles behave qualitatively as expected, they also illustrate, quite nicely, the rapid change in neutron spectrum that occurs at various locations throughout the excore regions.

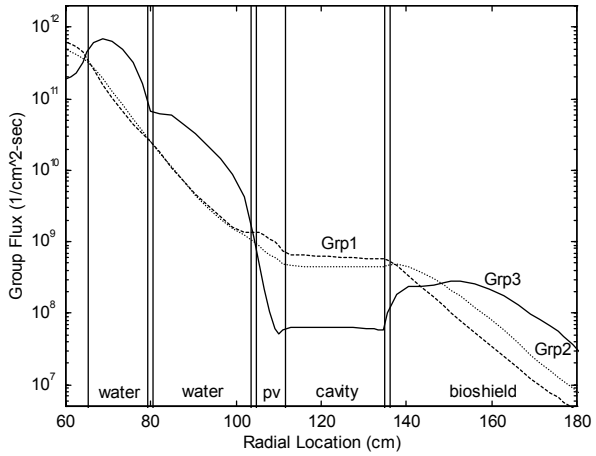

Fig. 3 JPDR broad-group radial flux profiles.

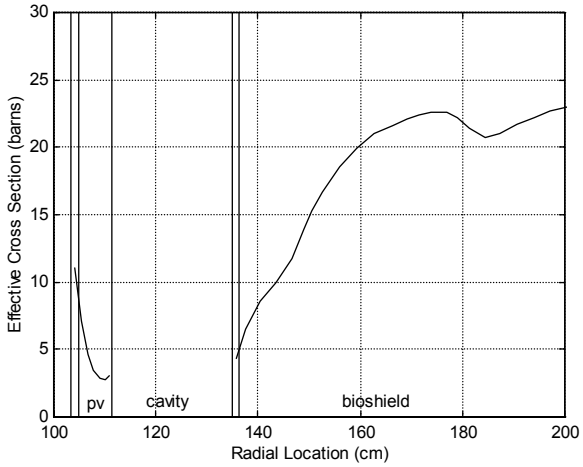

Fig. 4 ^{59}Co 1-group n,γ cross section profile.

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 good example is given in Fig. 4 which shows the effective ^{59}Co n,γ cross section versus radial position at an axial height of 360 cm. Note that the 1-group average cross section varies by about a factor of 4-5 in the two regions shown in Fig. 4 (pressure vessel and bioshield regions). 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.

IV. ACTIVATION ANALYSIS RESULTS

Using the 47-group fluxes from the DORT cases and the 47-group activation cross sections in ACTXS47.LIB, ACTIV was run using only the most important reactions that affect the nuclides of interest. The current calculations focused on the activities associated with ^{54}Mn, ^{55}Fe, ^{60}Co, ^{63}Ni, ^{152}Eu, and ^{154}Eu because these were measured as part of the experimental program in the JPDR. The activity of ^{134}Cs was also measured at selected locations within the bioshield, however, its parent isotope, ^{133}Cs, is not available in the current VITAMIN-B6 library. Therefore, the activity associated with ^{134}Cs could not be included in this study.

The abundances and decay data used in this study came directly from the ORIGEN data libraries[6] and the initial parent concentrations for the structural materials were taken from Table 2 of Ref. 2. The power versus time history for the ACTIV calculation was also taken from Ref. 2, Fig. A.4. There were ten alternating periods of constant power operation and full shutdown, with the last shutdown period lasting 15 years. This latter time interval represents the time from when the reactor was shutdown permanently to when the activation measurements were made. The total simulation time, from initial startup of the JPDR to the measurement time, was 10011.8 days.

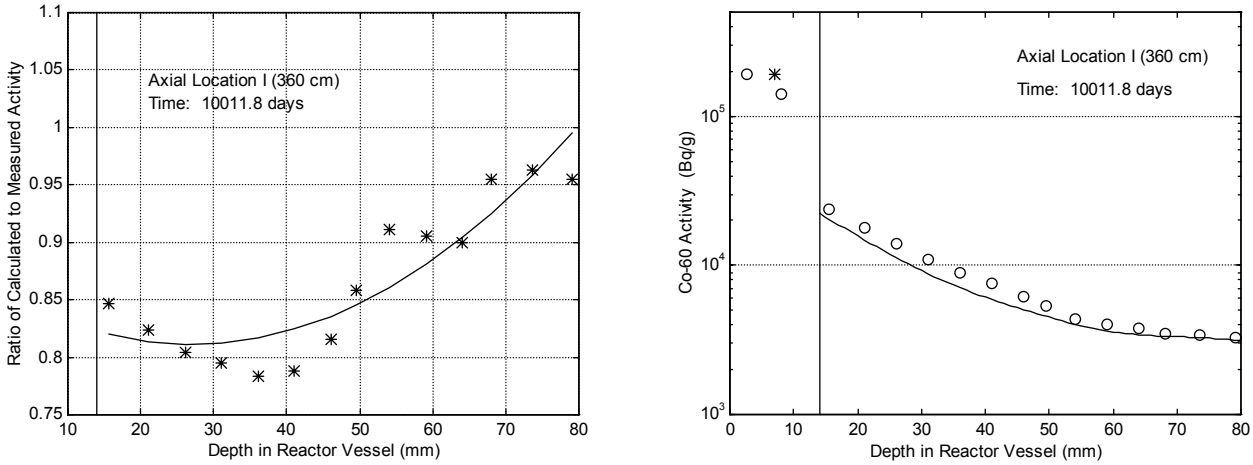

Fig. 5 ^{60}Co activity and C/E profiles within the reactor vessel.

With all this background to establish the specifics of the computations that were performed, we can now address the actual results of the study. The summary comparisons given here focus only on the radial ^{60}Co activity profiles, but all the other results in the benchmark study show similar behavior. In particular, Figs. 5 and 6 give the final comparisons of the measured and computed ^{60}Co radial activities using the 47-group DORT fluxes. Each figure comparing the calculated and experimental radial activities 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 (see Fig. 5), a quadratic fit was used and, in the bioshield (see Fig. 6), a simple linear fit was used.

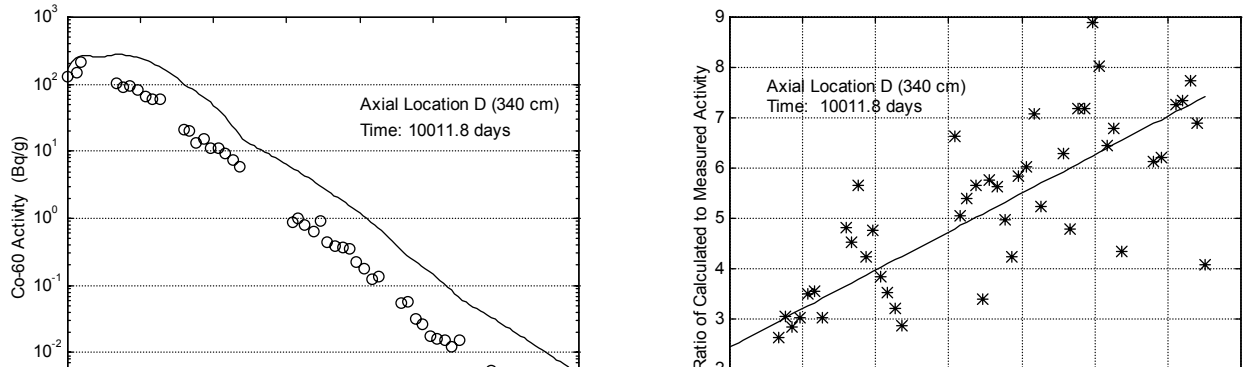

Fig. 6 ^{60}Co activity and C/E profiles within the bioshield.

Concerning the plots, one can easily argue that very good results were obtained for all points through the pressure vessel. For example, for the data shown in Fig. 5, the maximum error is less than 25%. This good agreement up through the vessel was also apparent in all the other radial and axial

activity profiles determined as part of this exercise. Thus, the overall accuracy of the calculations, up to and including the vessel, is on the order of ±25%. This is a very impressive finding, especially considering the complexity of the calculations required to produce these comparisons.

Figure 6, however, shows that this same level of accuracy is not achieved in the bioshield region. The calculation over predicts the measured activity at all points in the bioshield, and the error tends to grow with distance into the shield, approaching a factor of about 6 at approximately 100 cm into the shield. This behavior is consistent for all the isotopes, and additional analyses show that the error trend is roughly linear with distance into the concrete region.

The root cause of the bioshield discrepancies has not been isolated explicitly, although a number of sensitivity studies (quadrature order, mesh spacing, concrete composition, energy resolution, etc.) have been performed. The discrepancy is probably due to a combination of factors, including some remaining uncertainty in the actual bioshield model. Further work is needed to address this concern.

On a positive note, a larger uncertainty with distance into the bioshield, although worrisome from a modeling and analysis viewpoint, is probably not of real concern in practice, since the activity levels are so low anyway. The ^{60}Co activity, for example, is reduced by about 6 orders of magnitude at 100 cm into the shield relative to the magnitude at the inner surface of the pressure vessel. Thus, for disposal and general decommissioning concerns, the activity of the concrete beyond the first 100 cm is negligibly small compared to other components in the system. A factor of 5-10 error in a negligibly small activity may not be of practical concern – but it sure does leave room for some further investigations.

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