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Comparison of transport cross-section data generated with BONAMI and TRANSX

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Abstract. This work compares the results of radiation transport calculations performed with VITAMIN-B7 cross section data to calculations performed with a similar library prepared with the TRANSX code. The bases for the comparisons include a simplified, one-dimensional PWR model and the industry standard H.B. Robinson Cycle 9 reactor dosimetry benchmark. Comparisons are also made with a modified TRANSX-generated library with enhanced background cross section data. The results show significant differences between VITAMIN and TRANSX-generated libraries through iron media.

1 Introduction

As operating licenses for commercial nuclear power plants continue to be extended, interest is growing in qualifying predictions of neutron exposure at locations that are farther from the core of the reactor. As applied to reactor vessel integrity evaluations, these new regions of interest are commonly referred to the “extended beltline” of the reactor vessel. Recent research undertaken to study extended beltline neutron exposure calculations [1] has found significant differences between calculated values of fast neutron (E > 1.0 MeV) flux and iron displacements per atom (dpa) rate generated with deterministic and Monte Carlo techniques for regions subject to significant neutron attenuation through iron media.

The deterministic-to-Monte Carlo radiation transport comparisons performed in [1] used the VITAMIN-B7 and BUGLE-B7 libraries [2] as a comparison basis. The VITAMIN and BUGLE libraries are widely-used multigroup cross section data libraries for ex-core radiation transport simulations. Current versions are based on ENDF-B/VII.0, while historical versions are based on ENDF/B-VI.3, ENDF/B-V, and ENDF/B-IV. The VITAMIN libraries are 199-neutron and 42-photon energy group libraries, and the BUGLE libraries are 47-neutron and 20-photon energy group libraries derived from VITAMIN. Questions have been raised [3,4] about the adequacy of the self-shielding treatment employed in the recent versions of the VITAMIN libraries (and, by extension, the BUGLE libraries), and the degree to which the processing techniques used to generate the VITAMIN libraries may bias the results of calculations that employ those libraries. Specifically, the smallest background cross section in the VITAMIN libraries (1 barn) is larger than the background cross section for natural iron (~0.2 barn for Fe-56). This is potentially significant because LWR pressure vessel steels are comprised almost entirely of iron.

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In addition, the weighting flux for the VITAMIN libraries is computed by the BONAMI code (part of the AMPX [5] code package) the using the following formulation:

$$W_\ell(E) = \frac{C(E)}{(\sigma_t(E)+\sigma_0)} \quad (1)$$

In Equation (1), $W_\ell(E)$ is the weighting flux, $C(E)$ is the smooth part of the flux shape, $\sigma_t(E)$ is the total cross section, σ_0 is the background cross section, and ℓ is the Legendre order. However, in the formulation of the Bondarenko method employed by NJOY [6] and associated codes from Los Alamos National Laboratory, the quantity in the denominator is raised to the power of $\ell + 1$. Therefore, in Los Alamos codes, a different weighting flux is used for the 0th and 1st Legendre orders.

The objective of this work is to determine to what degree the issues outlined above affect transport calculation results for representative LWR pressure vessel neutron exposure problems. This is done by preparing a multigroup cross section library using ENDF-B/VII.0 [7] nuclear data in the same energy group structure as the VITAMIN libraries using the NJOY and TRANSX [8] codes. The new library, together with the VITAMIN-B7 library, are benchmarked against continuous energy Monte Carlo radiation transport results on a one-dimensional geometry representative of a PWR pressure vessel fluence model. Finally, two libraries prepared using TRANSX with differing minimum background cross sections and the VITAMIN-B7 library were used to analyze the H.B. Robinson Cycle 9 reactor dosimetry benchmark [9].

2 Nuclear data processing

The NJOY code sequence was used to process the evaluated nuclear data into a multigroup representation†. NJOY calculations were performed for the constituent isotopes of PWR fuel, water, boron, stainless and carbon steels, air, and concrete. A NJOY input template was prepared, and a Python script was used to populate inputs for each isotope. ENDF/B-VII.0 data were processed into the VITAMIN neutron and photon energy group structure at multiple temperatures, with background cross sections ranging from 1E+10 barns to 0.001 barns. A separate library was also prepared with minimum background cross sections of 1 barn to isolate the effect of the insufficiently small background cross section for Fe-56 in VITAMIN.

Using the NJOY outputs, the TRANSX code was used (in a manner analogous to the BONAMI code) to generate self-shielded material mixtures at specific temperatures and produce cross sections suitable for discrete ordinates radiation transport calculations. The TRANSX code is no longer maintained by Los Alamos National Laboratory. Version 2.15 is distributed via RSICC. Updates to TRANSX were developed [10] as part of work performed by the IAEA. For the current effort, the updates from [10] were applied, and additional cosmetic and array sizing updates were added. The consolidated set of updates used herein are available from the author of this paper.

† The `maxb` parameter in `matxsr.f90` was increased from 30000 to 300000. This allows the MATXSR module of NJOY to process larger outputs from the GROUPR module of NJOY.

3 Transport calculation comparisons

3.1 One-Dimensional Model Comparisons

A one-dimensional model of a PWR was prepared in MCNP [11] and DORT [12]. The model geometry is depicted in Figure 1, and the neutron source, materials, and temperatures were assigned consistently. The core neutron source was a spatially-uniform U-235 fission spectrum. In the case of the MCNP model, the energy distribution was sampled from 640-bin representation of the U-235 fission spectrum to capture the detailed shape of the fission spectrum. The MCNP calculations were performed in continuous energy mode.

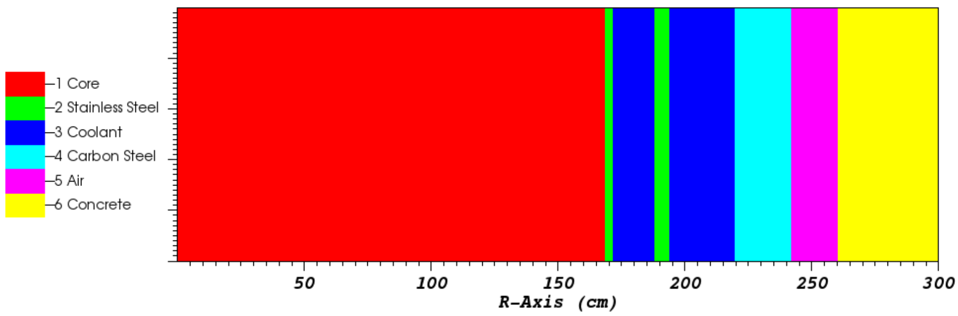

Fig. 1. One-Dimensional Monte Carlo PWR Model Used for Cross Section Benchmarking.

Neutron spectra were extracted/tallied in the VITAMIN 199-neutron energy group structure at the inner radius of the reactor pressure vessel (RPV) and at the outer radius of the RPV. The Monte Carlo uncertainties are negligible.

Comparisons of response functions computed by DORT (with the VITAMIN-B7 and TRANSX-generated libraries) and MCNP are shown in Table 1. Comparisons between the neutron spectra calculated by DORT and MCNP for the RPV inner radius appear in Figure 2 and Figure 3, while similar comparisons for the RPV outer radius appear in Figure 4 and Figure 5. All Figures only depict energies above 100 keV, which are the neutron energies usually most germane to material damage correlations.

Table 1. Ratio of Computed Response Functions (MCNP/DORT) for the One-Dimensional Problem.

	RPV IR VITAMIN-B7 Library	RPV IR TRANSX-Generated Library	RPV OR VITAMIN-B7 Library	RPV OR TRANSX-Generated Library
Flux (E > 1.0 MeV)	1.04	1.03	1.11	0.99
Iron dpa/s	1.03	1.03	1.09	0.97
Flux (E > 0.1 MeV)	1.04	1.04	1.09	0.96
Flux (E < 0.414 eV)	1.07	1.09	1.02	0.99

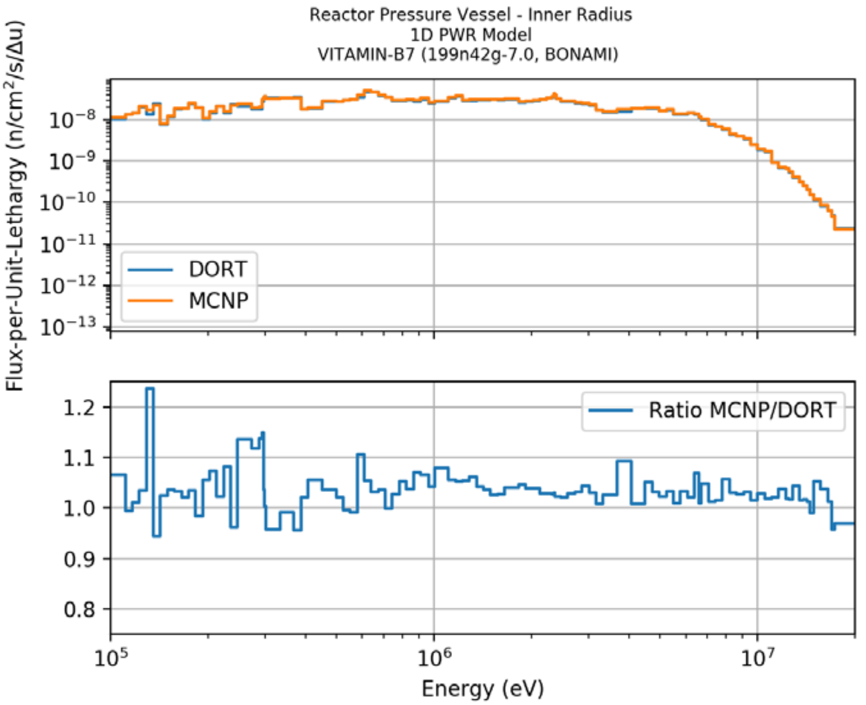

Fig. 2. Comparison of DORT (VITAMIN-B7 Library) and MCNP Results at the RPV Inner Radius.

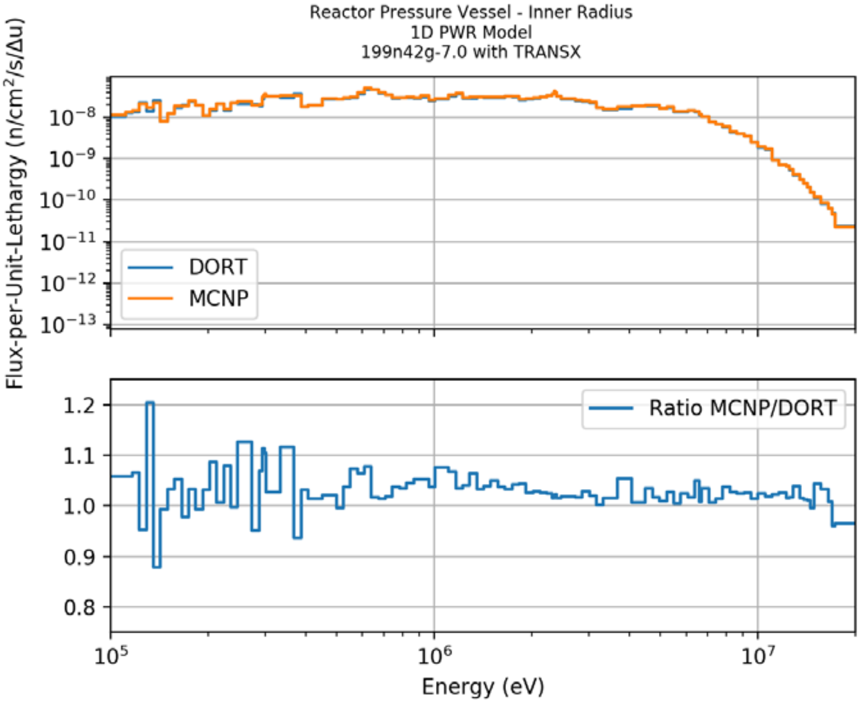

Fig. 3. Comparison of DORT (TRANSX-Generated Library) and MCNP Results at the RPV Inner Radius.

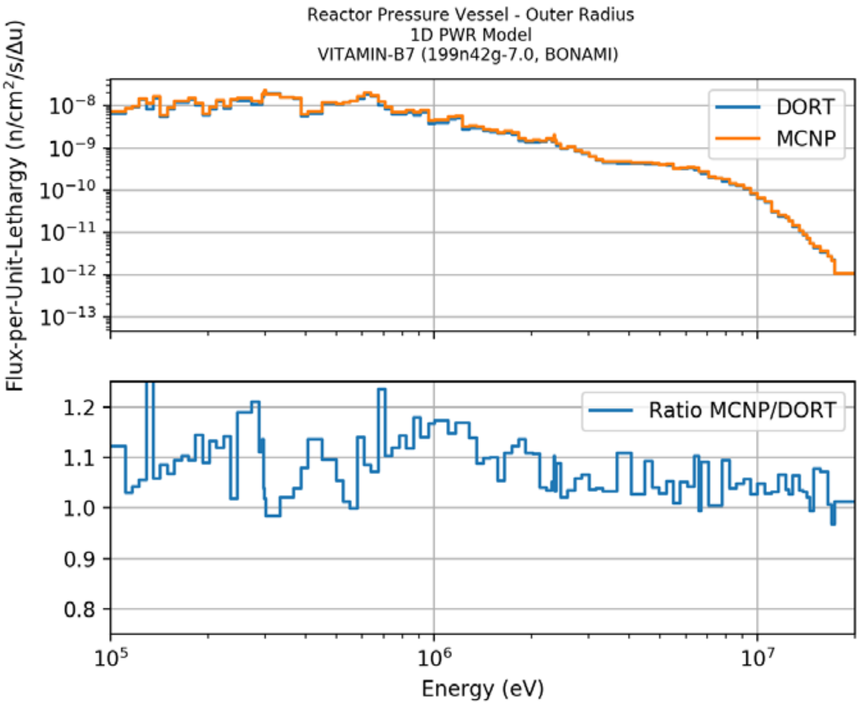

Fig. 4. Comparison of DORT (VITAMIN-B7 Library) and MCNP Results at the RPV Outer Radius.

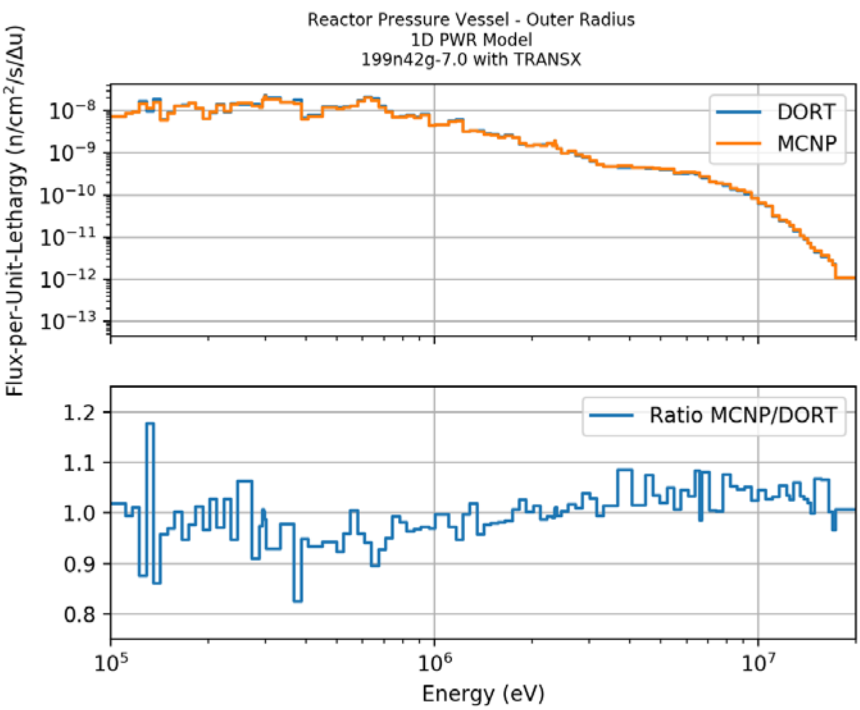

Fig. 5. Comparison of DORT (TRANSX-Generated Library) and MCNP Results at the RPV Outer Radius.

Table 1 and Figures 2 through 5 show that calculations based on both the VITAMIN-B7 and TRANSX-generated libraries show similarly good agreement with MCNP results at the inner radius of the RPV. However, at the outer radius of the RPV, the calculations based on the VITAMIN-B7 library show a deterioration in the level of agreement with MCNP, consistent with what was previously reported in [1], while the calculations based on the TRANSX-generated library maintains considerably better agreement with the MCNP results.

3.2 H. B. Robinson Cycle 9 Comparisons

Cycle 9 from H. B. Robinson Unit 2 was evaluated with the VITAMIN-B7 and the TRANSX-generated libraries to provide an additional comparison that is more representative of typical RPV fluence calculations. Cycle 9 at H. B. Robinson Unit 2 is an industry standard calculational benchmarking exercise [13]. These calculations were performed with a three-dimensional discrete ordinates radiation transport code, RAPTOR-M3G [14].

Comparisons of integral exposure parameters obtained from calculations employing the VITAMIN-B7 and TRANSX-generated libraries at the core midplane elevation are shown in Figure 6 for Fast Neutron (E > 1.0 MeV) Flux. The results based on the TRANSX-generated library produced higher flux values. At the surveillance capsule location, TRANSX-based values are 3% higher, at the RPV outer radius location, TRANSX-based values are approximately 20% higher. A similar results were observed with the iron dpa/s response function.

To test the effect of insufficiently small Fe-56 background cross section, a modified TRANSX library was prepared with a minimum cross section of 1 barn. A comparison of Flux (E > 1.0 MeV) results obtained from the reference and modified TRANSX-generated libraries at the core midplane elevation appears in Figure 7. At the surveillance capsule location, the libraries show no difference, and at the RPV outer radius location, the reference TRANSX-based values are approximately 5% higher.

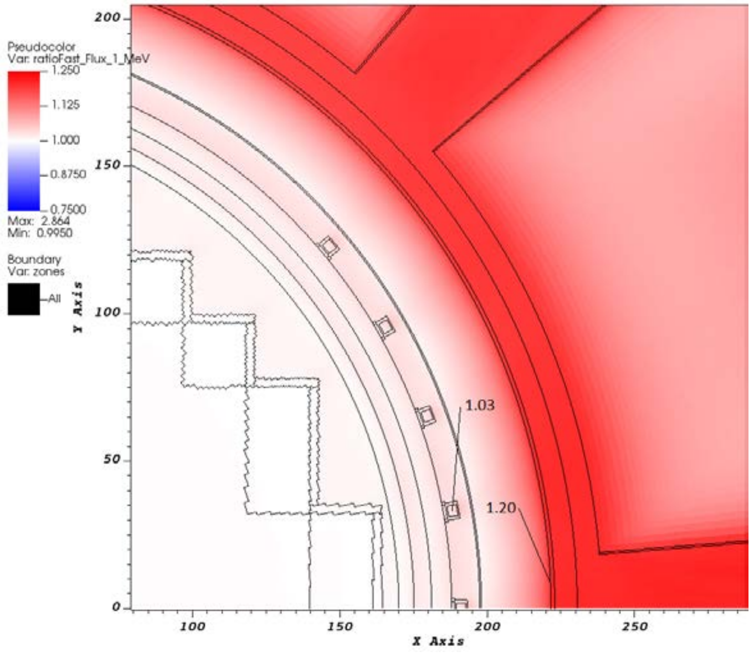

Fig. 6. Computed Flux (E > 1.0 MeV) Ratio (TRANSX-Generated/VITAMIN-B7) for H. B. Robinson-2 Cycle 9.

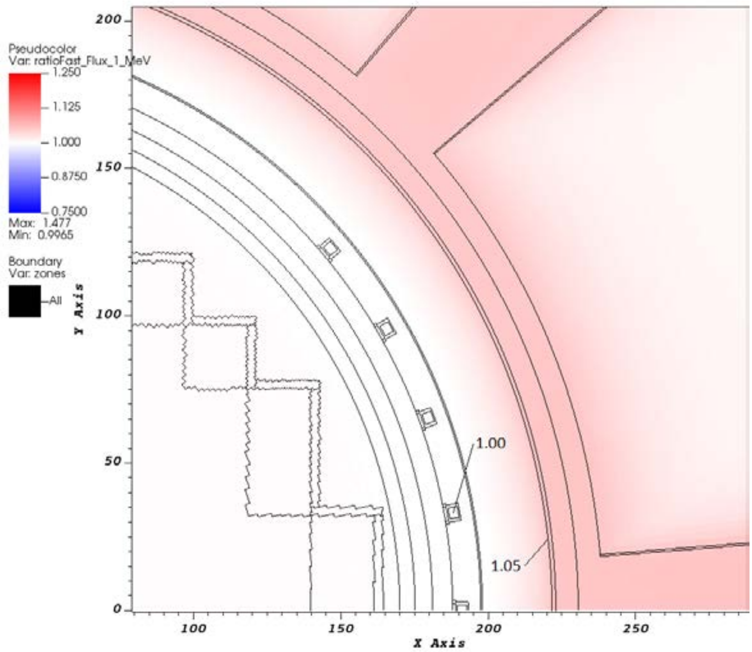

Fig. 7. Computed Flux (E > 1.0 MeV) Ratio (TRANSX-Generated/TRANSX$_{1b}$-Generated) for H. B. Robinson-2 Cycle 9.

4 Conclusions

Deterministic transport calculations employing cross sections processed with TRANSX and including reduced background cross sections for iron show significantly improved agreement with MCNP results on the exterior surface of RPVs as compared calculations performed with the VITAMIN-B7 library on the one-dimensional benchmark problem that was evaluated. Comparisons performed with the H. B. Robinson benchmark problem show that the differences largely result from the different formulations for the weighting flux employed by TRANSX versus BONAMI. These results suggest that deterministic methods can show good agreement with MCNP results, even in challenging situations such as neutron attenuation through iron media.

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