Use of the WIMS-E Lattice Code for Prediction of the Transuranic Source Term for Spent Fuel Dose Estimation

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USE OF THE WIMS-E LATTICE CODE FOR PREDICTION OF THE TRANSURANIC SOURCE TERM FOR SPENT FUEL DOSE ESTIMATION

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ABSTRACT

A recent source term analysis has shown a discrepancy between ORIGEN2 transuranic isotopic production estimates and those produced with the WIMS-E lattice physics code. Excellent agreement between relevant experimental measurements and WIMS-E was shown, thus exposing an error in the cross section library used by ORIGEN2.

I. INTRODUCTION

The planned re-racking of N Reactor fuel assemblies and packing of scrap into multiple canister overpack (MCO) containers has generated some concern as to the size of the spontaneous neutron source term, important in characterizing the estimated dose. Previous calculations using the RADNUC code (an automated interpolator code using ORIGEN2 production tables) has possibly over-estimated the size of the ^{244}Cm contribution by over an order of magnitude. The overall over-estimation of the source term may be at least a factor of five; this will result in greater (and unnecessary) expense in shielding requirements.

The ORIGEN2 computer code uses effective one-group cross sections in its burnup equations. These cross sections must come from somewhere, and various libraries exist for different applications. At least one existing ORIGEN2 library uses cross sections extracted out of older WIMS-D calculations; another library (for ORIGEN-S) was created specifically for N Reactor MKIV and MKIA inners and outers, using the Oak Ridge SCALE system.

The latest version of WIMS-E, version 6a, has recently been obtained from the British AEA Technology. This latest version of the code comes with the latest cross section library (1994) and comes in both 69 and 172 energy groups. This cross section library was created from the latest cross section evaluations from the Joint European File (JEF2.2), from ENDF-B/VI, and for the first time, includes extension of the transuranic burnup equations into the curium chains.

Preliminary results from WIMS-E 6a show a much smaller quantity of ^{244}Cm produced than the earlier ORIGEN calculations. In addition, WIMS-E 6a isotopic predictions for irradiated MKIV fuel (both inner and outer) are in excellent agreement with measured isotopic production data.[1]

In an attempt to upgrade ORIGEN2 capabilities for burnup analysis of N Reactor fuel types, new effective one-group microscopic cross sections have been extracted out of WIMS-E output for both MKIV and MKIA inners and outers as a function of burnup.

It is beleived that the discrepancy in the ^{244}Cm production is due to an error in the extraction of the one-group cross sections out of the earlier WIMS-D results.

II. ISOTOPIC PRODUCTION CALCULATIONS

The WIMS-E 6a computer code[2] was used in a burnup mode for both MKIV and MKIA N Reactor fuel types. Hot operating conditions (temperatures, thermally expanded dimensions and reduced densities) were taken from the DCODE fuels performance code, used extensively in the past in support of fuel design and operation of the N Reactor. To estimate the transuranic isotopic distribution of the spent fuel inventory, a database is required that contains information on the quantity of initial uranium metal and the total exposure present in each of the groups of spent fuel. A small FORTRAN post-processor program was written to extract the isotopic data out of the WIMS-E output files, and combine this data with the exposure

database. For every exposure group, the database contains the quantity of uranium metal and the exposure it has acquired. The WIMS-E production tables give the isotopic quantities (e.g., gram per metric ton of initial uranium) as a function of exposure. The post-processor takes an exposure group and uses a three-point interpolation to calculate the grams per metric ton of each isotope at that exposure, and multiplies this by the initial uranium in the group; the result is the total quantity of each isotope, for each group of spent fuel.

As a conservative estimate for the source term prediction, the highest-exposure 270 MKIV fuel assemblies (five tiers of 54 assemblies each) were assumed to be loaded into a single MCO. To treat non-linearities of isotopic quantities with burnup, it was decided to approximate these 270 fuel assemblies by equal mass quantities of MKIV fuel, each at five different exposures. The MKIA basis was 288 fuel assemblies (six tiers of 48 assemblies each). A FORTRAN program was used to interpolate the transuranic isotopics for each of the exposure bins, and sum over the five (or six) bins to find the total.

III. CALCULATION VALIDATION

Transuranic isotope quantities have been measured and documented for known burnups.[1] WIMS-E isotopic predictions agree very well for all of the isotopes that were compared. WIMS-E performs a cylindrical integral transport calculation in 69 neutron energy groups and then uses the transport solution to provide fluxes that drive the burnup equations in each burnable material. This is repeated for each burnup steps. WIMS-E therefore predicts the fraction of power (and exposure) produced in the inner and outer elements of the tube-in-tube geometry of N Reactor fuel. Power sharing ratios represent the ratio of either inner or outer element specific power (power per unit mass) to the assembly average specific power. These ratios are burnup dependent. Figure 1 shows how these ratios change with burnup; these values are consistent with the power sharing ratio assumed in the older ORIGEN model. Figures 2 and 3 illustrate the ^{235}U depletion in MKIV inner and outer elements, as predicted by WIMS-E and as measured. Figures 4 and 5 show the same comparison for ^{236}U buildup; the WIMS-E calculation assumed an initial ^{236}U content of 400 ppm. The plutonium isotope comparisons are shown in Figures 6 through 15.

Further along the burnup chain are the curium isotopes. Figures 16 and 17 show predicted ^{244}Cm contents for both inner and outer elements. The agreement is very good.

Figure 1. Power Ratio vs Exposure.
MKIV assemblies.

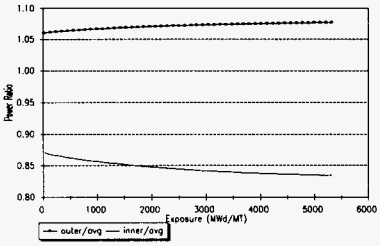


Figure 2. U-235 vs Exposure.
N Reactor MKIV Inner.

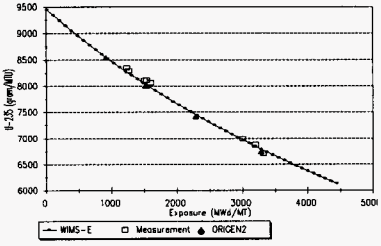


Figure 3. U-235 vs Exposure.
N Reactor MKIV Outer.

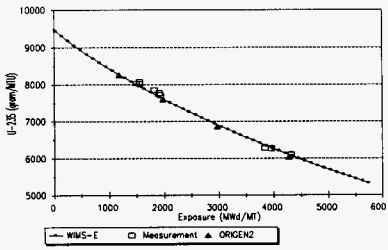


Figure 4. U-236 vs Exposure.
N Reactor MKIV Inner.

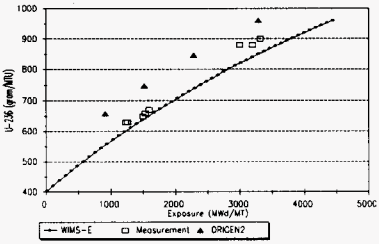


Figure 5. U-236 vs Exposure.
N Reactor MKIV Outer.

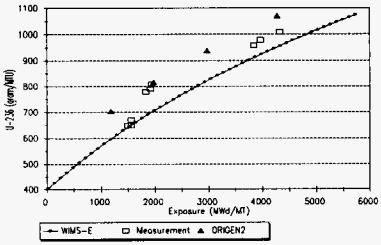


Figure 6. Pu-238 vs Exposure.
N Reactor MKIV Inner.

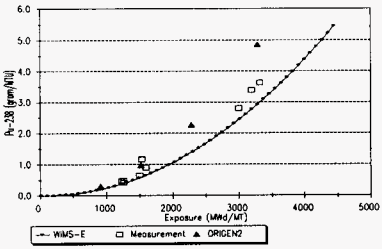


Figure 7. Pu-238 vs Exposure.
N Reactor MKIV Outer.

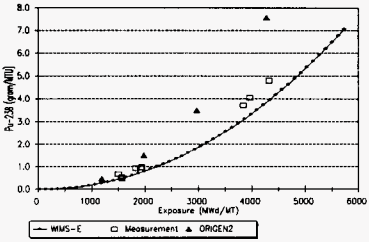


Figure 8. Pu-239 vs Exposure.
N Reactor MKIV Inner.

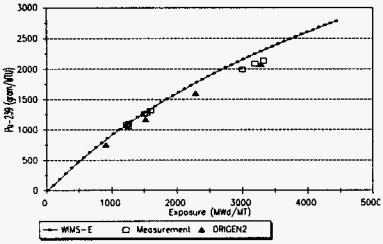


Figure 9. Pu-239 vs Exposure.
N Reactor MKIV Outer.

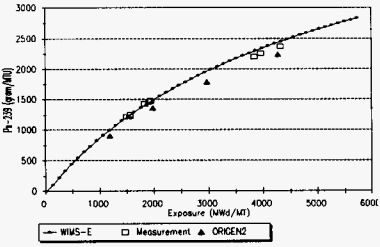


Figure 10. Pu-240 vs Exposure.
N Reactor MKIV Inner.

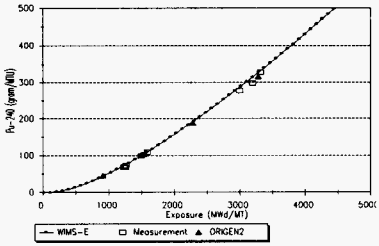


Figure 11. Pu-240 vs Exposure.
N Reactor MKIV Outer.

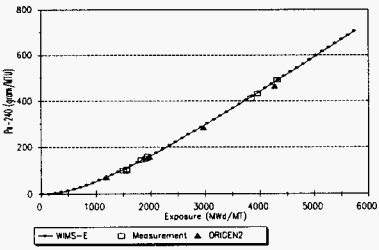


Figure 12. Pu-241 vs Exposure.
N Reactor MKIV Inner.

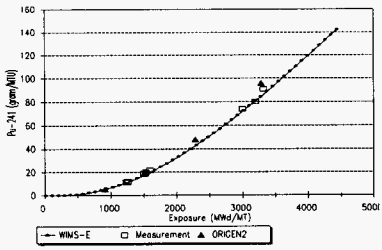


Figure 13. Pu-241 vs Exposure.
N Reactor MKIV Outer.

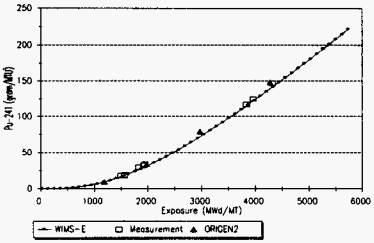


Figure 14. Pu-242 vs Exposure.
N Reactor MKIV Inner.

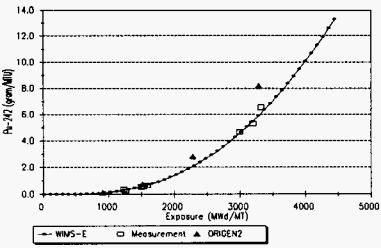


Figure 15. Pu-242 vs Exposure.
N Reactor MKIV Outer.

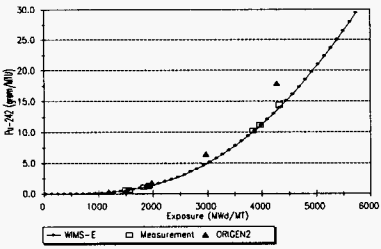


Figure 16. Cm-244 vs Exposure.
N Reactor MKIV Inner.

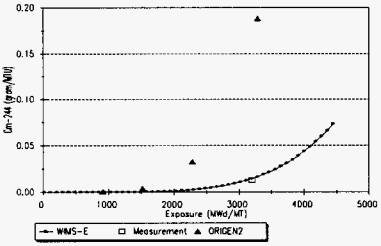
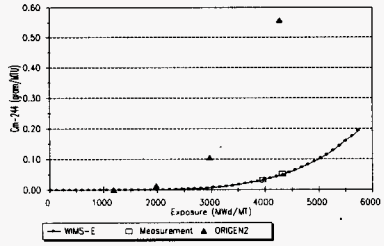


Figure 17. Cm-244 vs Exposure.
N Reactor MKIV Outer.



IV. EFFECTIVE ONE-GROUP CROSS SECTIONS

The effective self-shielded one-group microscopic cross section is defined by the equation:

$$\bar{\sigma}_x = \frac{\sum_{g=1}^{G} \sigma_{x,g}\phi_g}{\sum_{g=1}^{G} \phi_g} \qquad (1)$$

In Equation, $\bar{\sigma}_x$ is the effective one-group microscopic cross section of reaction type x. The 69-group neutron flux spectrum, ϕ_g, is used as the weighting function to average the microscopic group-dependent cross section, $\sigma_{x,g}$. The summation in the numerator is performed automatically by using the reaction rate output edit module W-WIRE, contained within the WIMS-E code. The summation in the denominator is simply the one-group neutron flux, and is output by using the W-WED module. A small FORTRAN program was written to read the ASCII text file produced by WIMS-E, and collect the data required to evaluate $\bar{\sigma}_x$. This post-processing was performed for both inner and outer elements, and for both MKIV and MKIA fuel types, as a function of burnup; 50 burnup steps were performed. Effective one-group cross sections were calculated for several uranium and transuranium isotopes, listed in the table below:

Nuclide Evaluated	WIMS-E ID code
^{235}U	2235
^{236}U	2236
^{238}U	2238
^{237}U	2237
^{237}Np	3237
^{239}Np	3239
^{238}Pu	4238
^{239}Pu	4239
^{240}Pu	4240
^{241}Pu	4241
^{242}Pu	4242
^{241}Am	5241
^{242m}Am	5242
^{243}Am	5243
^{243}Cm	6243
^{244}Cm	6244

The final set of effective one-group microscopic cross sections was delivered for modification of the ORIGEN2 cross section library.

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1. Wittekind, W. D., *Fuel Segregation Detector Calibration and DCODE Computer Modeling*, UNI-2384, UNC Nuclear Industries, Inc., Richland, Washington (1984).

2. Gubbins, M. E., M. J. Roth, and C. J. Taubman, *A General Introduction to the Use of the WIMS-E Modular Program*, AEEW-R 1329, Reactor Physics Division, AEE Winfrith, England (1982)