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MONTE-CARLO BURNUP CALCULATION UNCERTAINTY QUANTIFICATION AND PROPAGATION DETERMINATION

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ABSTRACT

Reactor burnup or depletion codes are used thoroughly in the fields of nuclear forensics and nuclear safeguards. Two common codes include MONTEBURNS and MCNPX/CINDER. These are Monte-Carlo depletion routines utilizing MCNP for neutron transport calculations and either ORIGEN or CINDER for burnup calculations. Uncertainties exist in the MCNP steps, but this information is not passed to the depletion calculations or saved. To quantify this transport uncertainty and determine how it propagates between burnup steps, a statistical analysis of multiple repeated depletion runs is performed. The reactor model chosen is the Oak Ridge Research Reactor (ORR) in a single assembly, infinite lattice configuration. This model was burned for a 150 day cycle broken down into three steps. The output isotopics as well as effective multiplication factor (k-effective) were tabulated and histograms were created at each burnup step using the Scott Method to determine the bin width. The distributions for each code are a statistical benchmark and comparisons made. It was expected that the gram quantities and k-effective histograms would produce normally distributed results since they were produced from a Monte-Carlo routine, but some of the results appear to not. Statistical analyses are performed using the χ^2 test against a normal distribution for the k-effective results and several isotopes including ¹³⁴Cs, ¹³⁷Cs, ²³⁵U, ²³⁸U, ²³⁷Np, ²³⁸Pu, ²³⁹Pu, and ²⁴⁰Pu.

INTRODUCTION

MONTEBURNS is a routine that links the Monte-Carlo Neutral Particle transport code (MCNP) with the Oak Ridge Isotope Generation and Depletion Code (ORIGEN 2.2) for burnup and depletion calculations (1). In the MCNP part of the routine, tallies are used to compute the total and six group neutron flux and reaction rates. The one group flux and reaction rates are then passed to ORIGEN through text files, along with isotopic information, which will compute the fission products, actinides, and activation products produced for the burnup step using the matrix exponential method (2) (3). MCNPX has the CINDER depletion routine as an option. Similarly to MONTEBURNS, MCNPX/CINDER alternates steps of transport and depletion calculations. Unlike the MONTEBURNS package, using CINDER does not require any additional input decks but the simple addition of a burn card in the MCNPX input. CINDER solves the series of linear differential equations using the Markov method; a statistical method in which decay chains are repeatedly sampled until convergence achieved (4).

There exists an uncertainty in each code's Monte-Carlo transport calculation which is not passed to the depletion routines or saved. A previous study determined that using enough histories to only satisfy MCNP statistical checks on reaction rates and flux tallies using MONTEBURNS resulted in greater than desired uncertainty in the output isotopics (5). Beginning with the quantity of histories to converge these tallies, MCNPX/CINDER and MONTEBURNS runs were performed 200 times

each at three different quantities of histories. Every run began with a different Monte-Carlo random seed to preserve randomness in the results. In addition to observing the uncertainty propagation through burnup steps, the reduction in uncertainty and propagation through adding additional histories was determined.

REACTOR MODEL DESCRIPTION

The ORR materials test reactor (MTR) fuel assemblies possess curved fuel plates which overlap in one dimension. To simulate an infinite lattice, a translation of part of the assembly must be done to preserve the correct assembly pitch. In this model, half of the assembly was translated and periodic boundary conditions were used in the X and Y dimensions. The fuel and burnup parameters are shown in Table I (6).

Table I. MONTEBURNS fuel and depletion parameters for ORR.

Parameter	Value	Parameter	Value
²³⁵ U Enrichment	93%	Burn Steps	3
Material Form	U ₃ O ₈	Decay Steps	2
Other U Isotopes	234, 236, 238	Full Fuel Volume [cc]	362.4
Cladding Material	Al	Full Assembly Power [MWt]	1.11
Side Plate Material	Al	Modeled Fuel Volume [cc]	6.040
Days Burned [d]	150	Modeled Power [kWt]	18.5

The fuel possesses a large quantity of ²³⁵U. When too much of an isotope is present in a model, the statistically varying digit and the round off digit may fall in the same place in the MONTEBURNS gram quantity output results. In previous work, this rounding of the statistically varying digits created an undesired set of binned results instead of a true normally distributed histogram (5). To avoid this and prevent rounding bias, the model was modified to be 1.0 cm in height and reflective boundary conditions were used.

BURN RESULTS

Due to the random nature of the Monte-Carlo process, this procedure was expected to produce results that formed a normal distribution. Three fission products, three uranium isotopes and 13 transuranic isotopes all shown in Table II were forcefully tracked during all runs.

Table II. Isotopes tracked for all runs.

Xe-135	U-238	Pu-241	Am-243
Cs-134	Np-237	Pu-242	Cm-242
Cs-137	Pu-238	Pu-244	Cm-243
U-234	Pu-239	Am-241	Cm-244
U-235	Pu-240	Am-242	-

The first isotope examined was ¹³⁵Xe with a short half-life of 9.1 h and a strong absorption cross section of 2×10^6 b. During a constant irradiation, it establishes an equilibrium concentration in about 1-2 days (5). Using MONTEBURNS, the ¹³⁵Xe average mass at the end of burnup step three, the

last full power step, was $1.30 \times 10^{-5} \text{g} \pm 1.99\%$, $1.30 \times 10^{-5} \text{g} \pm 0.535\%$, and $1.30 \times 10^{-5} \text{g} \pm 0.212\%$ for 5000, 75000, and 375000 histories respectively. A similar reduction in uncertainty was observed using MCNPX/CINDER with $1.20 \times 10^{-5} \text{g} \pm 1.74\%$, $1.20 \times 10^{-5} \text{g} \pm 0.421\%$, and $1.20 \times 10^{-5} \text{g} \pm 0.206\%$ for 5000, 75000, and 375000 active histories respectively. The results from both codes are plotted in Figure 1. The decrease in uncertainty is as expected from the additional histories and follows Poisson statistics. As the uncertainty is lowered, an even greater quantity of additional histories is required for further reduction.

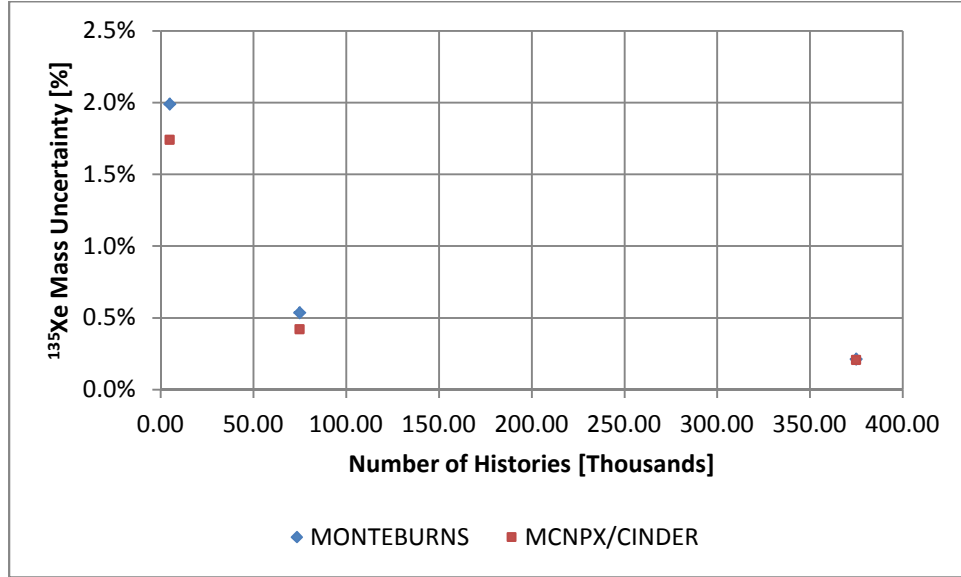


Figure 1. ¹³⁵Xe mass uncertainty reduction as the quantity of histories increases.

Statistically, the two codes converged to different ¹³⁵Xe quantities which may be attributed to differences in the flux between the two models as they each handle transport calculation's isotope importance threshold differently (1) (4). This may be avoided by forcing both codes to track a set of approximately 140 isotopes at every step; severely penalizing CPU time for multiple or repeated runs.

¹³⁷Cs was examined next to show the reduction in uncertainty in histogram form. At the end of step five, MONTEBURNS resulted with $9.56 \times 10^{-2} \text{g} \pm 0.787\%$, $9.55 \times 10^{-2} \text{g} \pm 0.210\%$, and $9.55 \times 10^{-2} \text{g} \pm 0.0832\%$ for 5000, 75000, and 375000 active histories respectively; while MCNPX/CINDER resulted with $9.72 \times 10^{-2} \text{g} \pm 0.653\%$, $9.71 \times 10^{-2} \text{g} \pm 0.148\%$, and $9.71 \times 10^{-2} \text{g} \pm 0.0676\%$. These results show a similar reduction in uncertainty as ¹³⁵Xe while adding additional histories. The three sets of results for MONTEBURNS are displayed in Figure 2. The histograms were created using the same bins to show convergence.

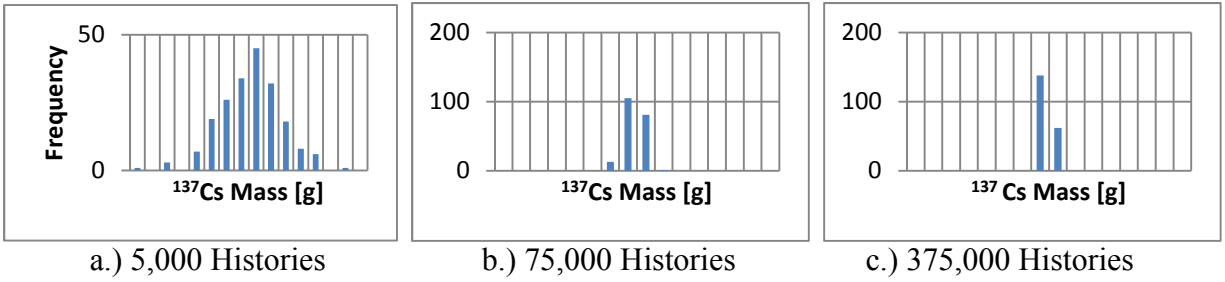


Figure 2. Histograms of ^{137}Cs results at the end of step 5 using MONTEBURNS.

The reactor initial uranium isotopics consisted of ^{234}U , ^{235}U , ^{236}U , and ^{238}U in the quantities shown in Table III. The uranium was in the form of U_3O_8 mixed with aluminum. The modeled fuel volume is $1/60^{\text{th}}$ the actual volume.

Table III. Initial Uranium Isotopics.

Isotope	Mass Percent [%]	Assembly Initial Mass [g]	Modeled Initial Mass [g]
^{234}U	0.2489	3.064	0.0511
^{235}U	23.16	285.1	4.751
^{236}U	0.1076	1.325	0.0221
^{238}U	1.347	16.58	0.2764

Of the initial four uranium isotopes, only ^{234}U , ^{235}U , and ^{238}U were added into both codes' output files. Similar to ^{135}Xe , the two codes' uranium results converged to statistically different quantities as a result of different fluxes and burnup due to the transport calculation's isotope importance threshold functioning differently. For most steps, the ^{234}U and ^{238}U uncertainties are lower using MONTEBURNS while the ^{235}U uncertainty is lower using MCNPX/CINDER. The tabulated ^{235}U results from MCNPX/CINDER are shown in Figure 3.

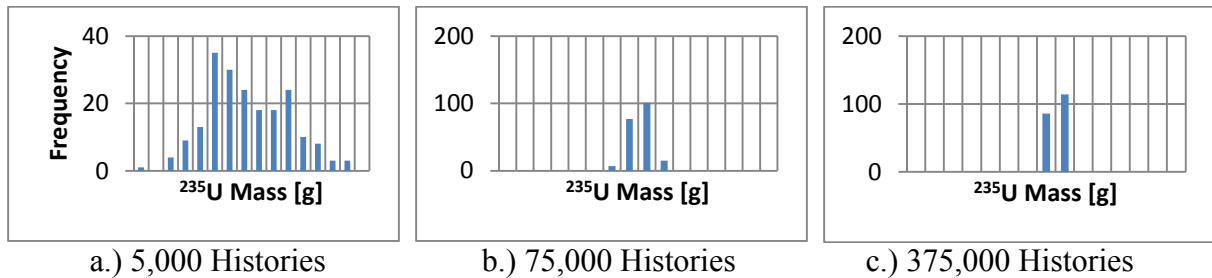


Figure 3. Histograms of ^{235}U results at the end of step 5 using MCNPX/CINDER.

The MCNPX/CINDER package only outputs four significant digits. In this model, the large quantity of ^{235}U causes minor round off effects where the statistically varying and round off digits fall in the same place. If a full histogram were created using the 375,000 active history results, the low uncertainty and round off effects may create false empty bins.

All of the isotope results from the final full power burn step, step 3, and final decay step, step 5, are summarized in Table V. Certain isotopes are expected to have the same quantity at step 3 and 5 due to very long half lives. The results show that for higher actinides the uncertainty generally increases as more absorptions and decays are required for production. It is expected that the uncertainty for the higher actinides would be greater due to lower quantities and longer production chains. With the exception of a few fission products, the MONTEBURNS uncertainties were generally lower than the MCNPX/CINDER uncertainties using the same quantity of histories. For fission products and uranium isotopes, the uncertainties were much closer but MCNPX/CINDER seemed to produce larger uncertainties overall.

Table IV. Summary of isotopic mass results at 375,000 histories at steps 3 and 5.

Code	MONTEBURNS	MCNPX/CINDER	MONTEBURNS	MCNPX/CINDER
Isotope	Step 3 [g]	Step 3 [g]	Step 5 [g]	Step 5 [g]
¹³⁵ Xe	1.298E-05 ± 0.212%	1.203E-05 ± 0.206%	0.000E-00 ± 0.000%	0.000E-00 ± 0.000%
¹³⁴ Cs	1.229E-02 ± 0.370%	1.256E-02 ± 0.350%	8.786E-03 ± 0.370%	8.976E-03 ± 0.349%
¹³⁷ Cs	9.775E-02 ± 0.083%	9.938E-02 ± 0.068%	9.552E-02 ± 0.083%	9.712E-02 ± 0.068%
²³⁴ U	3.075E-02 ± 0.218%	2.695E-02 ± 0.215%	3.083E-02 ± 0.217%	2.703E-02 ± 0.215%
²³⁵ U	1.415E+00 ± 0.183%	1.368E+00 ± 0.161%	1.415E+00 ± 0.183%	1.368E+00 ± 0.161%
²³⁸ U	2.367E-01 ± 0.067%	2.386E-01 ± 0.083%	2.367E-01 ± 0.067%	2.386E-01 ± 0.083%
²³⁷ Np	3.915E-02 ± 0.503%	3.604E-02 ± 0.646%	4.568E-02 ± 0.513%	4.211E-02 ± 0.656%
²³⁸ Pu	9.416E-03 ± 0.534%	9.540E-03 ± 0.670%	1.004E-02 ± 0.531%	1.016E-02 ± 0.663%
²³⁹ Pu	7.115E-03 ± 0.522%	6.588E-03 ± 0.684%	8.102E-03 ± 0.523%	7.537E-03 ± 0.698%
²⁴⁰ Pu	2.793E-03 ± 0.672%	2.764E-03 ± 0.765%	2.796E-03 ± 0.671%	2.767E-03 ± 0.766%
²⁴¹ Pu	3.298E-03 ± 0.400%	3.141E-03 ± 0.529%	3.143E-03 ± 0.400%	2.993E-03 ± 0.530%
²⁴² Pu	1.764E-03 ± 0.508%	1.741E-03 ± 0.545%	1.764E-03 ± 0.508%	1.741E-03 ± 0.545%
²⁴⁴ Pu	1.267E-06 ± 0.845%	2.673E-07 ± 1.030%	1.267E-06 ± 0.845%	2.673E-07 ± 1.030%
²⁴¹ Am	1.225E-05 ± 0.447%	1.067E-05 ± 0.566%	1.670E-04 ± 0.400%	1.585E-04 ± 0.530%
²⁴² Am	2.229E-07 ± 0.479%	6.448E-08 ± 0.610%	2.219E-07 ± 0.479%	6.416E-08 ± 0.610%
²⁴³ Am	3.431E-04 ± 0.810%	2.604E-04 ± 1.013%	3.462E-04 ± 0.810%	2.628E-04 ± 1.014%
²⁴² Cm	8.602E-06 ± 0.477%	1.012E-05 ± 0.667%	1.864E-06 ± 0.475%	2.178E-06 ± 0.665%
²⁴³ Cm	1.556E-07 ± 0.663%	1.848E-07 ± 0.841%	1.519E-07 ± 0.663%	1.803E-07 ± 0.843%
²⁴⁴ Cm	9.576E-05 ± 0.840%	7.806E-05 ± 1.040%	9.233E-05 ± 0.840%	7.631E-05 ± 1.040%

The mean k-effective and standard deviation for steps 0, 3, and 5 are shown in Table V. Since every step uses the same quantity of histories, it was expected that the code's output uncertainty in each step's k-effective would be similar. For the statistically calculated standard deviations, uncertainty arises in the ²³⁵U quantity and the k-effective distribution flattens and spreads outward which is seen in Figures 4 and 5.

Table V. k_{eff} results for both codes.

Code	Step	5000 Histories	75000 Histories	375000 Histories
MONTEBURNS	0	$1.783 \pm 0.369\%$	$1.783 \pm 0.0864\%$	$1.783 \pm 0.0385\%$
MCNPX/CINDER	0	$1.787 \pm 0.348\%$	$1.786 \pm 0.0940\%$	$1.786 \pm 0.0422\%$
MONTEBURNS	3	$1.366 \pm 0.727\%$	$1.366 \pm 0.170\%$	$1.366 \pm 0.0799\%$
MCNPX/CINDER	3	$1.283 \pm 0.766\%$	$1.284 \pm 0.187\%$	$1.284 \pm 0.0836\%$
MONTEBURNS	5	$1.381 \pm 0.730\%$	$1.383 \pm 0.176\%$	$1.384 \pm 0.0872\%$
MCNPX/CINDER	5	$1.268 \pm 0.838\%$	$1.269 \pm 0.184\%$	$1.269 \pm 0.0875\%$

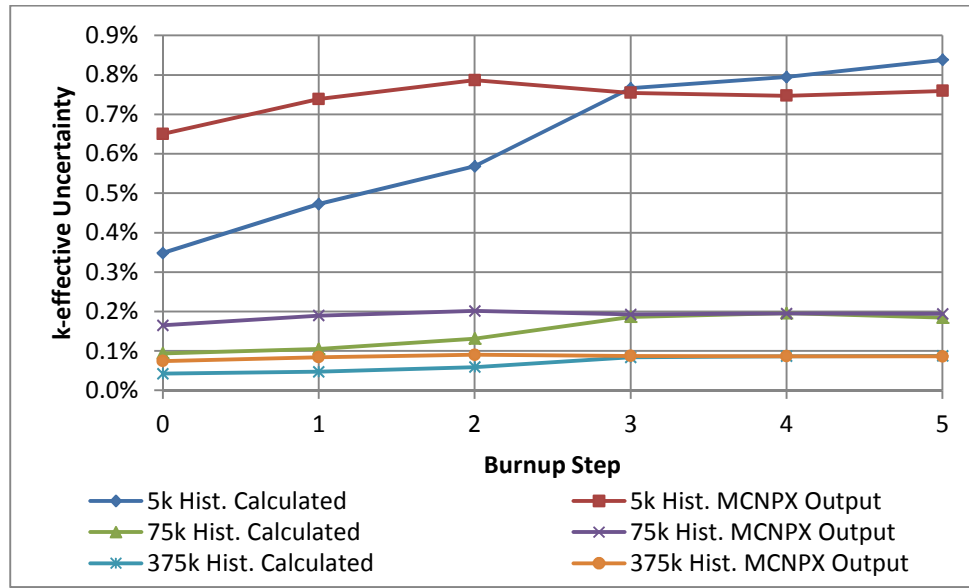


Figure 4. MCNPX k_{eff} uncertainty results.

The MCNP output uncertainty was consistent in every step for a given run. The standard deviation was calculated from 200 repeated runs at each burnup step. This began lower than the MCNPX output and propagated to be equal or greater than it. If many more burnup steps are used, the k -effective uncertainty may propagate to be statistically larger than the MCNPX reported calculation and must be taken into consideration for more complicated power histories. The same effects arose with the MONTEBURNS runs.

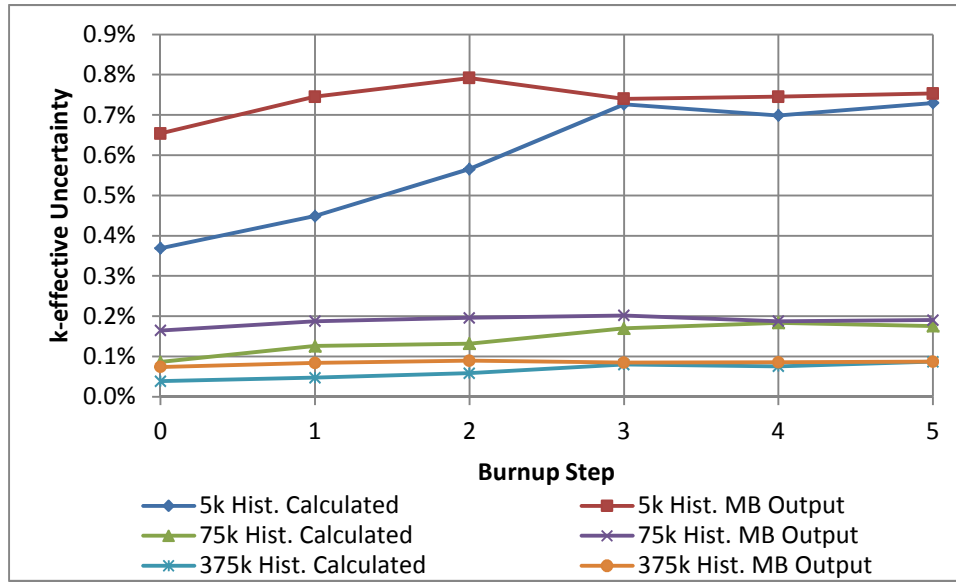


Figure 5. MONTEBURNS k_{eff} uncertainty results.

STATISTICAL TESTS

To test if the results were normally distributed they were tested against a normal distribution using the χ^2 test at α of 0.05. These tests were performed using 14 bins with 11 degrees of freedom since two parameters are estimated. The null hypothesis in these tests is that the distribution is normal. The results of these tests for ^{137}Cs after burnup step 3 are shown in Table VI. The test statistic was compared to the χ^2 value of 19.68 for all tests.

Table VI. χ^2 distribution tests for ^{137}Cs after step 3.

Histories	MONTEBURNS χ^2 Statistic	Reject Null ($\alpha=0.05, \chi^2 < 19.68$)	MCNPX/CINDER χ^2 Statistic	Reject Null ($\alpha=0.05, \chi^2 < 19.68$)
5000	15.49	No	9.735	No
75000	8.889	No	9.389	No
375000	5.951	No	12.78	No

In the MONTEBURNS results, the χ^2 statistic was reduced as the number of histories increased. The MCNPX/CINDER χ^2 statistic did not have the same strong reduction effect, but all three tests failed to reject the null hypothesis. The same test was done on the mass distributions for ^{239}Pu with 375000 histories at all full power burnup steps. The results are shown in Table VII.

Table VII. χ^2 distribution tests for ^{239}Pu using 375000 histories.

Step	MONTEBURNS χ^2 Statistic	Reject Null ($\alpha=0.05, \chi^2 < 19.68$)	MCNPX/CINDER χ^2 Statistic	Reject Null ($\alpha=0.05, \chi^2 < 19.68$)
1	12.46	No	6.593	No
2	8.886	No	6.995	No
3	13.39	No	11.27	No

While some of the histograms do not make these distributions appear to be normal, the null hypothesis that the distribution is normal is failed to be rejected in each step. This same test was performed on ^{235}U , in which all six tests failed to reject the null hypothesis as well.

Statistical tests on k-effective were also performed using the results from 5000 and 375000 histories with both codes. Although both codes have capabilities of creating mid-step k-effective calculations, the statistical tests were performed on the end of step results. The null hypothesis failed to be rejected at every step from both codes. The results from the MCNPX/CINDER χ^2 tests are shown in Table VIII. In a previous study, the χ^2 statistic grew as uncertainty propagated through burnup steps. Comparing these results to this study, the χ^2 statistic growth can be mainly attributed to round off which was primarily eliminated from this study.

Table VIII. χ^2 distribution tests for k_{eff} using MCNPX/CINDER.

Step	5000 Histories χ^2 Statistic	Reject Null ($\alpha=0.05, \chi^2 < 19.68$)	375000 Histories χ^2 Statistic	Reject Null ($\alpha=0.05, \chi^2 < 19.68$)
0	6.383	No	6.428	No
1	14.14	No	7.373	No
2	13.60	No	8.114	No
3	10.35	No	12.33	No
4	8.183	No	13.59	No
5	8.239	No	8.193	No

CONCLUSIONS

The Monte-Carlo depletion codes MONTEBURNS and MCNPX/CINDER possess an uncertainty in its reaction rate and flux tallies. This information is not passed on or propagated through the burnup calculations. A statistical analysis to examine and understand this uncertainty as well as its effect on variation in isotope generation and depletion was performed. A simple infinite lattice assembly level model of the ORR was burned using 3 burnup steps and 2 decay steps in 200 separate runs using different random number seeds. These results created a distribution of k-effective and fission products. This process was performed using 5000, 75000, and 375000 active histories with each code.

To examine a greater accuracy solution using MONTEBURNS, the results were created using nine significant digits as opposed to the default three. Of these nine digits only five of them are of value because the flux solution has only five digits. Using the same quantity of histories, MONTEBURNS produced lower uncertainties in the output isotopes for the majority of actinides. MCNPX/CINDER and MONTEBURNS had statistically similar uncertainties for the fission products tested with MCNPX/CINDER's being slightly lower. Due to differences in the two code's transport calculation isotope importance, the fluxes and burnup were not the same. This can be corrected by forcing each code to add approximately 140 isotopes to the transport calculation at every step but has a severe penalty to runtime.

Statistic analyses of these distributions were performed against a normal distribution using the χ^2 test. The k-effective and isotope mass distributions all failed to reject the null hypothesis that the distribution is normal. These results suggest that if severe round off is avoided by controlling the

quantity of each tracked isotope and using enough histories to satisfy the MCNP internal statistical checks, the resulting k-effective and isotope mass distributions are statistically normal.

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