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REACTOR FUEL DEPLETION BENCHMARK OF TINDER

W. J. Martin
Sandia National Laboratories
PO Box 5800, MS-1136, Albuquerque, NM 87185-1136
wjmarti@sandia.gov

ABSTRACT

Accurate burnup calculations are key to proper nuclear reactor design, fuel cycle modeling, and disposal estimations. The TINDER code, originally designed for activation analyses, has been modified to handle full burnup calculations, including the widely used predictor-corrector feature. In order to properly characterize the performance of TINDER for this application, a benchmark calculation was performed. Although the results followed the trends of past benchmarked codes for a UO_2 PWR fuel sample from the Takahama-3 reactor, there were obvious deficiencies in the final result, likely in the nuclear data library that was used. Isotopic comparisons versus experiment and past code benchmarks are given, as well as hypothesized areas of deficiency and future work. *

Key Words: Burnup, Depletion, Nuclear Reactor, CINDER2008, TINDER

1. INTRODUCTION

Concerns with nuclear waste disposal, high burnup nuclear reactor fuels, and advanced reactor designs have made accurate, high-fidelity depletion calculations a high priority in order to properly predict the end-state of a variety of systems. Thankfully, over the last half century, several computer codes have been developed and maintained to directly get at this goal[1–6]. These codes, however flexible, have been tailored over the years for their current applications – namely light water reactors (ORIGEN) and accelerators/particle physics (CINDER). This somewhat narrow scope has limited the features of these codes to only neutron-induced reactions and to purpose weighted multigroup transmutation reaction libraries. Therefore, in order to accurately model all aspects of the concerned areas, either modifications need to be made to existing codes or new codes must be developed.

The latter option would involve starting from the beginning in terms of programming but utilizing the existing experience base. New efforts to do this have approached the problem in a different way than the past depletion codes. For example, the Serpent[7] Monte Carlo reactor physics code has included burnup integrally in the the transport code. This allows for the same Doppler-broadened and self-shielded nuclear data to be used in both the transport and burnup calculations without having file communication between codes or modules. One other feature that is a great improvement over the main-stream codes is the on-the-fly multiple burn zones within single materials and pins, throughout an entire assembly and core. Typically this sort of zoning would require thousands of manual definitions of materials and zone, but can now be done with a single command.

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Although these new codes have many of the features that have been lacking in the previous codes, they still need benchmarking, verification and validation, and traction in the nuclear community. Additionally, these codes are still heavily in development and are not complete. It is therefore also useful to modify existing codes to have a much wider scope.

An example of modifying an existing code has been seen with the CINDER2008 code from Los Alamos National Laboratory[3]. This modified version allows for not only neutron-induced transmutation reactions to be tracked, but also those that are photon-induced[8]. With long-life and high burnup reactor cores, the marginal photon-induced transmutation reactions possibly could cause meaningful depletion and activation. Additionally, as a feature of the CINDER2008 code, cross-section libraries can be easily created using any source of ENDF-B/6 formatted data, allowing for any multigroup structure, weight function, and self-shielding method to be used. This new tool allows for the data to be made consistent with the data used in the transport calculation and reality.

The TINDER code has been introduced previously as a wrapper program to couple CINDER2008 and any transport codes for use with activation analyses[8]. As activation and depletion analyses are extremely similar, modifications have been made to the TINDER code to handle full burnup calculations. This code coupling allows for full reactor burnup calculations to be performed while not only tracking neutrons and photons in the transport calculation, but also while carrying them through the transmutation portion as well. A benchmark study is therefore necessary in order to qualify this new code suite for use in this fashion.

The following section, Section 2, gives brief details on the methodology used in the TINDER wrapper in terms of burnup. The benchmark calculation is described in Section 3.1 with the results and summary of that calculation given in Sections 3.2 and 3.3. Finally, conclusions and future work are outlined in Sections 4 and 5.

2. METHODOLOGY

TINDER is a wrapper code that allows for automated communication between the dual particle version of CINDER2008 and nearly any neutral particle transport code–so long as the code can return volume averaged fluxes. A typical TINDER run consists of calling the transport code to get the initial state of the flux, then passing that information to CINDER2008 for the depletion step. The resulting material compositions and delayed photon signal are then passed back to be used in the subsequent transport and transmutation steps. As this interface has been detailed in other publications, this paper will simply address the new burnup routine that has been added[8].

The burnup routine used in TINDER allows for several of the typical features found in similar codes. These features include a predictor-corrector routine that can be turned on or off (to maintain the applicability of TINDER for activation and decay problems), a constant power approximation that can change at each burn step, and an on-the-fly bookkeeping for the materials in the libraries of the transport and burnup codes. In short, TINDER creates the necessary files for and calls the transport and transmutation codes, and outputs the information in a consistent and transparent structure, including summary files as well as all individual program output files.

The first main feature of the TINDER burnup routine is the optional predictor-corrector routine.

The algorithm used in TINDER was modeled after the routine in a similar wrapper code, MCODE[9]. The first step in the process is to run an initial transport calculation to determine the beginning state of the system. This calculation gives the start of time step flux, which is then used in the predictor depletion for the current step. This depletion is run for the full length of the time step to determine the predicted end-state of the system. These projected materials are then fed into the predictor flux calculation for the step to make an estimate of the end-state flux of the system. When the predictor-corrector routine is not selected, these predictions are used as the final estimate for the timestep and these steps are repeated for all remaining timesteps.

If the predictor-corrector routine was chosen, the corrector step begins by taking an average of the flux values from the previous and predictor calculations. This flux is then fed into a depletion calculation as done before (using the beginning-of-step material quantities) and burned again for the full time step. These corrected end-of-step materials are then sent back to the transport calculation for a final corrected transport calculation. This process is then repeated, using the newly calculated final flux as the input flux for the next step, until all time steps have been completed.

This process yields beginning- and end-of-step values for all pertinent information. As of the current version of TINDER, the pertinent information that is summarized by the program output includes the k_{eff} of the system and the material inventories at each step. This algorithm for the predictor-corrector does not yield timestep averaged values for this information. Figure 1 gives a flow chart representation of the burnup routine in TINDER.

The second feature that is important for burnup calculations that has been added to TINDER is the constant power approximation for each timestep. In fact, this feature has always existed in CINDER2008, but was not utilized by the TINDER wrapper algorithm prior to the burnup additions. This feature allows for a constant power to be produced from the burned material by iterating on a flux normalization factor until the fission power produced from the system is equal to the desired power (within a given tolerance).

Finally, on-the-fly bookkeeping is handled by TINDER. As the large number of isotopes with decay data in CINDER2008 and the likely smaller number of isotopes with cross-sections in the transport code will be generally mismatched, TINDER seamlessly translates the material identifications from one code to the other and keeps track of those that may be missing from the smaller library. This enables CINDER2008 to keep track of all burned materials accumulating over the burnup history, even if they are not used in the transport calculation. The data library in CINDER2008 used for this effort contains approximately 4100 isotopes, 1325 isotopes describing the 120 fission product yield sets (60 neutron-induced and 60 photon-induced fission), and approximately 425 isotopes with cross-section information.

3. RESULTS

3.1. Benchmark Details

In order to ensure TINDER is a viable tool for burnup calculations, comparisons to benchmarks must be made. As experimental benchmark data is available, it is best to compare against that instead of attempting a simple code-to-code verification.

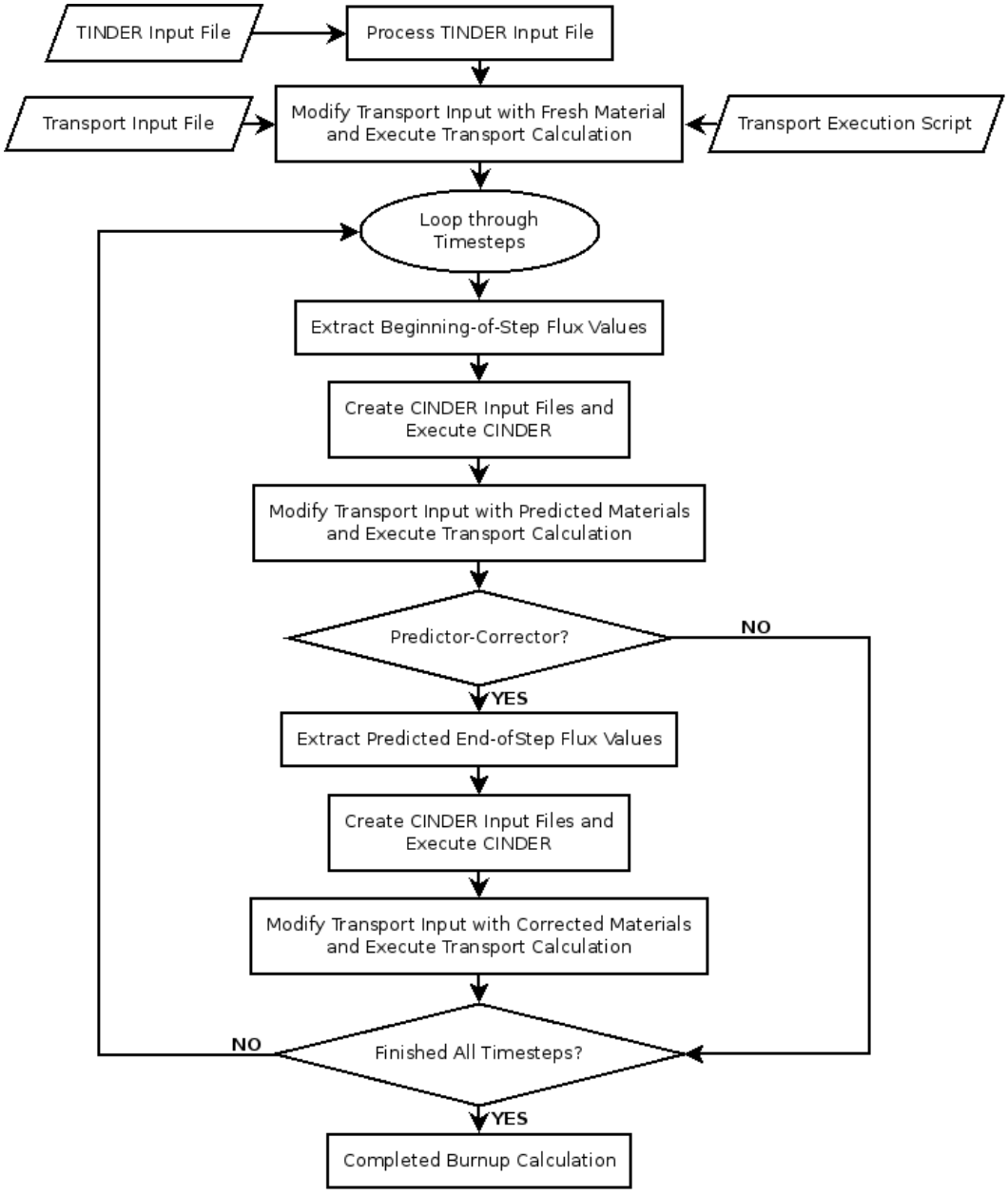

Figure 1. Predictor-corrector algorithm currently used in TINDER for burnup calculations.

One such experimental benchmark set of data for burnup comes from the Takahama-3 reactor in Japan[10]. Several samples with different burnups and compositions were taken from several axial and radial locations within a fuel assembly. These samples were then tested to determine the burnup level (using ^{148}Nd analysis) and isotopics. The original report, although written in Japanese, was later translated into English[11] for benchmark calculations performed on the SCALE code package[12,13].

For this current benchmark, a single sample is compared. Sample SF-95-4 was taken from a corner rod in the 17×17 assembly, furthest away from the burnable poison and control rods, at slightly above the axial mid-plane. This U(4.11%)O_2 sample saw a total burn-up of 36.69 GWd/MTU during two full cycles in the reactor. Additionally, a detailed power history was provided for the individual sample in the original and subsequent reports[10,11,13]. A final detailed composition of the fuel sample is also given for comparison. Figure 3.1 shows the cross-sectional location of the fuel sample in assembly SF-95. Geometric symmetries were taken advantage of to enhance the statistics in the 2-dimensional, full assembly model. Therefore, each corner rod was used in the tally for the neutron and photon fluxes to pass to the transmutation calculation.

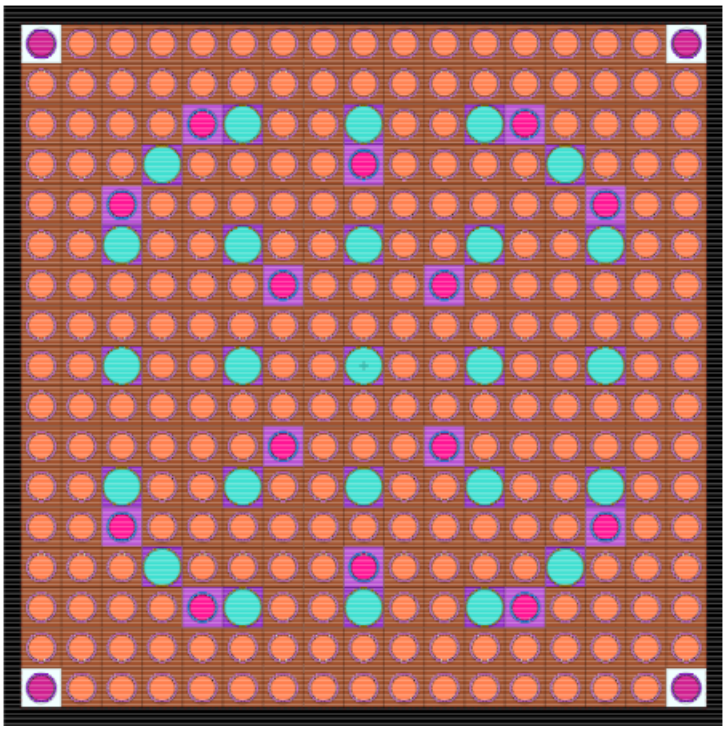

Figure 2. Cross-sectional view of the Takahama 17×17 PWR assembly. The sample position is located in each corner, highlighted by pink fuel and white coolant. Orange colored rods are standard fuel pins, light blue rods are water holes, and pink with blue rods are burnable poison pins.

The Monte Carlo particle transport code MCNP6-beta2[14] was used to perform the transport portion of the burnup calculation. The geometry was simplified from a full 3-D assembly model

to a 2-D assembly model that was infinite in the axial direction. In the other directions, the model is reflected. This model is in line with the simplified models used in the original benchmark which simply modeled each axial sample location as an independent 2-D slice[13]. Each KCODE transport step was performed with 200 active cycles after source convergence (approximately 50 inactive cycles), 5000 source particles per history, and using the coupled neutron/photon mode. F4 tallies were utilized for both neutrons and photons in the sample location cells to get volume averaged fluxes.

TINDER automatically processed these fluxes and transferred them to the CINDER2008 calculation. The detailed time power history was used for the full burnup as given in Table 6 of the report by Sanders and Gauld[13]. For the first 8 day cycle, the time steps were broken into much smaller steps to enable better characterization of the reactor start-up. Subsequent steps were taken in single passes, where no single powered step was greater than 50 days in length. Additionally, it was assumed that there was no cooling at the end of life for the final isotopic comparison.

3.2. Benchmark Results

Since this benchmark fuel was untouched during the full power irradiation history, only the end of life isotopic composition is known. Therefore, this is the single point of data that is used in the comparison to the code results. As mentioned, it was assumed for the code calculation that there was no cooling time after irradiation and before post irradiation examination was performed. This would greatly affect the results of short-lived isotopes and their products, so only stable or long-lived isotopes were used for the comparison.

In addition to comparing against the experimental data, the report by Sanders and Gauld includes results for two other codes, the SAS2H and HELIOS codes[13]. The performance of these codes is included as a point of reference to ensure that the TINDER calculation, if it differed from the experiment, it still was in line with other calculations.

The comparison to experiment is done by the standard, simple ratio of the calculation to the experiment, or C/E. A C/E of 1 is desired as this would mean that the code predicted the identical result that was measured, while a C/E of greater or less than 1 would imply that the code over or under predicted the final mass, respectively. Table 3.2 gives these ratios for the current benchmark.

Overall, TINDER performed similar to the other code benchmark results, which are generally in line with the experimental results. The fission product results for ^{106}Ru, ^{125}Sb, cesium, neodymium, and ^{154}Eu are somewhat similar to past results, where the over and under prediction of the final masses are consistent. In some cases, like ^{142}Nd and ^{144}Nd, TINDER's results are significantly lower than both the experiment and the earlier predictions. This discrepancy could be the result of the fission product spectra used in CINDER2008, which was not updated with the transition from CINDER90, or it could be caused by discrepancies in the decay data for fission products that include these isotopes in their decay chains.

The predicted mass results for the uranium isotopes are much closer to the experimental data, with slight deviations coming in the less abundant ^{234}U and ^{236}U. Likely, this is caused by poor estimation of the resonance self-shielding that is included in the multigroup cross section data for

Table I. Selected isotopic prediction comparisons of the Takahama-3 reactor benchmark for fuel sample SF95-4 after a burnup of 36.69 GWd/MTU. The TINDER results were produced using MCNP6-beta2 as the transport solver. The SAS2H and HELIOS results are repeated from [13] for comparison.

ISOTOPE	SAS2H	HELIOS	TINDER	ISOTOPE	SAS2H	HELIOS	TINDER
Ru106	1.27	1.25	1.34	U236	1.00	1.00	1.08
Sb125	2.60	2.88	2.71	U238	1.00	1.00	0.99
Cs134	0.86	0.82	0.34	Pu238	0.97	0.99	0.49
Cs137	0.99	0.97	0.97	Pu239	0.97	1.02	2.07
Ce144	1.05	1.00	1.03	Pu240	1.02	1.01	1.79
Nd142	0.88	-	0.50	Pu241	0.95	1.00	0.81
Nd143	0.98	0.98	1.08	Pu242	1.02	0.92	0.44
Nd144	0.98	0.96	0.84	Am241	1.54	1.45	1.35
Nd145	1.01	1.00	1.07	Am242m	1.05	1.03	-
Nd146	1.01	1.00	0.95	Am243	1.18	1.01	0.08
Nd148	0.99	0.99	1.02	Cm242	0.52	0.75	0.31
Nd150	0.99	0.98	1.04	Cm243	0.78	0.77	0.34
Eu154	0.95	1.04	0.68	Cm244	0.96	0.91	0.05
U234	1.27	1.01	1.82	Cm245	0.58	0.87	0.01
U235	0.98	1.00	1.21	Cm246	0.88	0.84	0.01

CINDER2008. An infinite dilution approximation was made when collapsing the resonances, which could cause the relative reaction rates to be misaligned.

The large discrepancies come in with some of the minor actinides, like plutonium and curium. As mentioned, the production rates for these isotopes may be off due to the approximation in the self-shielding of the cross sections. Although this may explain the slight problems with the estimates of plutonium and ^{241}Am, it is likely not enough to explain the extremely poor results for all the curium and remaining americium isotopes, which must be investigated further.

3.3. Benchmark Summary

Overall, although the trends in the results for TINDER did match those of the previous modeling benchmark efforts, there were large discrepancies in some fission products and the majority of the actinides. These results point to deficiencies in the proper modeling and simulation of the system. It is hypothesized that although some of the problem may be caused by poor fission product yield data, the main issue is in the handling of the resonance self-shielding. Improper estimates of the self-shielding factor that should be used have the potential to change the reaction probabilities for

individual isotopes, potentially over-emphasizing capture or fission reactions for example.

One note is that this benchmark was performed only on one single sample from the available 16 given in the initial report[10,11]. A more complete comparison and benchmark of the TINDER could be performed using these other samples. Sanders and Gauld performed the benchmark against all samples, providing a full set of results for the SAS2H and HELIOS codes as well[13].

4. CONCLUSIONS

The TINDER code has been modified to perform reactor burnup calculations. An initial benchmark of the code additions was made using experimental data and previous benchmark results of other burnup codes for a PWR UO_2 fuel sample from the Takahama-3 reactor.

Although the results as predicted by TINDER were consistent with those from SAS2H and HELIOS, there were large discrepancies. Overall, the parts averaged being off by 49%, with the median being 42%. This is most likely due to the nuclear data library in CINDER2008. The infinite dilution approximation made when performing the resonance self-shielding likely caused the resonances to be over-emphasized in the multigroup library, which in turn likely caused reactions reactions like (n,xn) to be under-emphasized in the final reaction rates. This would account for the large discrepancies in the actinide concentrations at the end of the irradiation history. Discrepancies in the fission products is likely due to the fission product yield data that was carried over from CINDER90.

In the end, TINDER proved to be a viable tool for burnup calculations of nuclear reactors. The code coupling with MCNP6 is handled seamlessly, but great care must be taken when selecting and processing the nuclear data for CINDER2008. Therefore, for TINDER use in everyday burnup calculations, data libraries should be benchmarked for certain application spaces to ensure the final results are useful.

5. FUTURE WORK

The logical next step is to benchmark TINDER further with other experimental data sets, including those from other facilities and reactor types. In doing so, the data should be checked at each step to ensure it is fully applicable to that environment.

Once the code has been benchmarked for standard problems, it should be expanded to allow for an arbitrary number of burn zones. Other improvements include quasi-parallel processing of the CINDER2008 calls (calling several instances at once) for multiple burn zones to enhance the speed of the calculation.

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