MODELLING BURNUP AT NRU LOOP SITES USING MCNP

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Abstract

NRU loop sites offer a unique irradiation capability to test fuel assembly performance at high flux and reactor operating temperatures. Accurate prediction of burnup at the scale of individual fuel pin-segments is a challenge in this highly heterogeneous environment, but must be pursued both to better interpret historic data, and to offer future clients more precise burnup time series.

Bundles with different geometries have at times been irradiated simultaneously, in many permutations, and new configurations might be of interest. The preparation of high-fidelity models of these configurations presents a challenge, as the model of the irradiation of a single string of six fuel bundles requires the composition and tracking of approximately 2000 cells. An automated model generation tool is discussed and preliminary simulation results presented.

1. Introduction

The National Research Universal (NRU) reactor at Chalk River, Ontario is a 100 MWth heavy water cooled and moderated core with hexagonal fuel channel layout. The heterogeneous design features an air-cooled graphite thermal column, annular light water reflector, driver fuel rods, absorbers, Mo-99 production assemblies, other irradiation facilities, and various beam tubes, etc. Low-enriched uranium driver rods occupy 80-90 of 227 lattice sites. Isotope production or other irradiation facilities occupy another 18-20 sites. The remaining sites are non-fueled.

Loop facilities U-1 and U-2 are a pair of independently cooled light-water circuits that extend through the core at three sites[2]. The loops are physically sized to approximate the pressure tubes of commercial pressurized heavy water reactors, and may be heated and pressurized to approximate those conditions. Six fuel bundles, modified to remove the center pin, are threaded onto a tie rod to form a *string* for irradiation. When operating, the loops are a significant reactor component, with thermal output per loop site on the order of a couple percent of reactor total.

A large variety of experimental fuels have been irradiated in the loops [1]. Trials have considered various pin sizes, mixture of sizes, number of pins, pin placement, pin composition, and fuels with composition that varies axially. Detailed breakdown of fuel burnup by pin and pin axial-segment is needed to assess irradiation performance of the trial fuels. Post-irradiation isotopic analysis is expensive and does not provide a detailed time series of the burnup. Simulation is conducted as an alternative.

[2] At one time there were five loop sites. Two have been decommissioned and, as of 1975, the U-2 loop facility occupies two sites in series.

Burnup of fuel in the loops has been historically simulated by BURFEL, [2], an in-house software package. For each pin-segment, a relative contribution to channel thermal output is determined according to,

$$contribution = thermal\ flux \times \frac{fission\ power}{nominal\ flux} \times \frac{coolant\ heating}{fission\ power} \tag{1}$$

Thermal flux is calculated from the site-specific axial distribution provided by the NRU neutron diffusion code TRIAD3. Particular units are not important, since results are later normalized. The *fission-power-to-nominal-flux ratio* is pre-computed depending on burnup of the bundle segment. The final term is the *power-to-coolant-ratio*, a fuel-specific constant. An additional correction is applied to account for end flux peaking [3]. The contributions are normalized so that the sum of all contributions, from all pin-segments in the loop site, equals the observed site thermal output. After normalization, the fission power of each pin-segment is determined from equation (1).

In validation tests against isotopic analysis, the BURFEL simulation scheme has been found to underestimate loop-string burnup on the order of 10%. Efforts to improve parameter estimates have not led to improved burnup estimates. Loop coolant circuit calorimetry has been repeatedly tested and found to be accurate. An improved physics model may be required.

An MCNP model of the entire NRU core is being developed as an evolutionary improvement, in an effort to identify biases in the BURFEL methodology. An MCNP model that includes each individual pin-segment may be used to estimate pin-segment burnup directly from tallies, thus avoiding arbitrary parameters.

Improved simulation of the loop fuel burnup will increase the utility of the large record of unique irradiations that have been conducted at NRU, and will provide customers with better results from future experiments. The work described here was carried out as a proof of concept toward such capability. A method to automatically include loop strings in the full-core NRU MCNP model was created. To do so consistently over a reasonably long period of time is a challenge due to the variety of bundle geometries that have been irradiated in the loops. Evaluation of MCNP for burnup purposes in NRU is beyond the scope of this paper, but the model generator described here was created with such future applications in mind.

2. Methodology

The existing MCNP model of NRU was extended to include the loop sites, as described in section 4, below. The model includes all fissionable rods and control devices. The outer structure of the model, excluding core sites, is shown in Figure 1. MCNP cards to describe driver fuel rods, Mo-99 production rods, absorber rods and loop fuel strings are generated automatically depending on the core loading. The initial burnup of individual rod segments and loop fuel bundles are copied from TRIAD3 and BURFEL. The burnup is updated for later timesteps according to the scheme below.

Burnable-material compositions are determined using pre-calculated depletion tables. WIMS-AECL 3.1 (WIMS-AECL) models of each individual rod or loop-bundle type are routinely used to generate neutronic data for TRIAD3 and BURFEL, with boundary represented as a moderator region. In these models, a constant thermal flux is specified on an intermediary surface between the fuel and the annular boundary-regions, and the boundary regions are given small fissionable and absorber content chosen to keep $k_{eff} \approx 1$. WIMS-AECL then conducts a depletion calculation at intervals of one to ten days over the residence time of the rod or bundle. The result is a table of fuel isotope composition (rows) by fuel burnup (columns).

MCNP5 version 1.40 was used to determine the neutron flux profile, and the relative fission power of individual fuel pins or groups of pins. An in-house patch of MCNP5 was used to examine the conversion from MCNP units of energy (MeV) into traditional units of burnup (MWh/kg IHE). This adjustment and the specific relation between tallies and burnup, are discussed in section 3, below. By attributing fission power to fissionable volumes over a timestep, new burnup values are determined, and an updated model can be created through the depletion tables. This process is repeated over the course of the irradiation of interest.

With the recent release of MCNP6, users now have the capability to conduct similar depletion calculations directly through the BURN card. The BURN card instructs MCNP6 to find a converged power distribution, invoke the CINDER90 depletion library for a time step, and then repeat as desired. This method is used for analysis of other research reactors [4]. Other depletion libraries may be used through a variety of external wrappers, such as MONTEBURNS for the ORIGEN-S library. BURNCAL, [5], is an interesting scheme that uses tallies to perform depletion calculations from explicit reaction rates. The choice in this study to continue using depletion tables from WIMS allows for a potential basis of comparison with BURFEL.

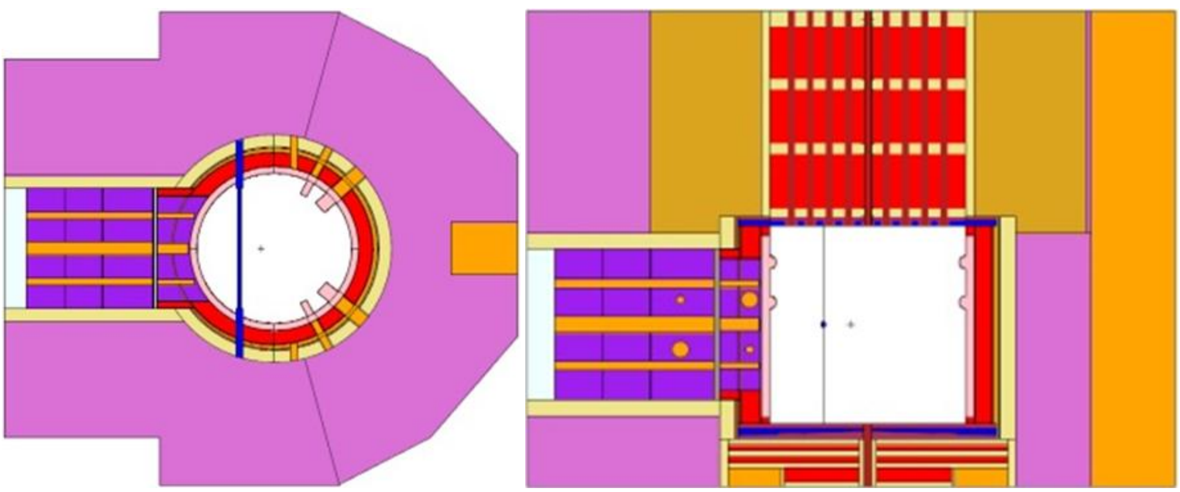

Figure 1 Cross-sections of the existing NRU model, showing reactor outer structure.

3. Calculation of Burnup

Total burnup of all fuels in the reactor is reliably measured as total reactor thermal output. The MCNP F7 tally accounts for energy release from fission, as a sum of fission q-values, in units of MeV, weighted by reaction rates and summed for specified volumes. These tallies can be related to traditional units of burnup according to,

$$Burnup\ Increment = \frac{Cell\ F7\ Tally}{Core\ F7\ Tally} \times \frac{Thermal\ Power\ Increment\ [\mathrm{MWh}]}{Cell\ Mass\ [\mathrm{kg\ IHE}]}. \qquad (2)$$

Table 1 compares the prompt and total fission q-values of the ENDF-B/VII MCNP libraries with the corresponding evaluation from WIMS-AECL. The WIMS-AECL library evaluation includes total fission energy, including decay products, and a constant 5.99 MeV/fission correction to account for parasitic neutron capture. This constant correction is validated for use with commercial pressurized heavy water reactors, and therefore may not reflect the appropriate level of neutron capture in NRU. To relate reactor thermal power output to cell burnup, as would be accounted for by WIMS-AECL, may require a unit conversion, according to,

$$Burnup\ Increment = \frac{Cell\ F7\ Tally\ [\text{WIMS MeV}]}{Core\ F7\ Tally\ [\text{WIMS MeV}]} \times \frac{Thermal\ Power\ Increment\ [\text{MWh}]}{Cell\ Mass\ [\text{kg IHE}]} \qquad (3)$$

Equations (2) and (3) should give nearly identical results if the ratios between WIMS-AECL q-values and prompt energy release q-values are nearly identical for those isotopes representative of most fission. QFISS (Q-values Fission) is a patch to MCNP developed by Atomic Energy Canada Limited that allows this hypothesis to be verified. The patch allows the user to modify the hard-wired MCNP fission q-values at runtime, affecting F7:n tallies exclusively [6].

Reaction Isotope	Prompt Energy Release MCNP table 98 default value, in MeV.	Total Energy Release MCNP reaction MT-318 default value, in MeV.	Total Recoverable WIMS ENDF/B VII evaluation, in MeV
U-234	179.45	191.84	197.590
U-235	180.88	193.48	202.356
U-236	179.50	194.49	202.346
U-238	181.31	198.03	204.489
Np-237	183.67	196.37	202.346
Pu-239	189.44	198.84	211.261
Pu-240	186.36	199.47	207.571
Pu-241	188.99	201.98	213.700
Pu-242	185.98	201.58	209.613

Table 1 Fission q-values of select isotopes.

4. Model Generation

An MCNP model of the full NRU core, excluding the loop sites, has been previously reported [7]. In this scheme, universe numbers and cell identifiers are carefully allocated among NRU core sites. A template file is loaded, to which fuel assemblies such as driver rods, Mo-99 production rods, or fast neutron rods are added. An additional spreadsheet with macros was created to be used in sequence with the existing full-core model. By way of comments added as a one-time modification to the initial template file, this new spreadsheet recognizes the specific cards associated with the loops.

In the present work, individual bundle models are provided as templates that are applied to the appropriate loop site and axial position. The spreadsheet reads the history of NRU rod changes to determine which loop-strings to load, determines the bundles within that string, then applies the appropriate template for each bundle. New cell, surface, material and tally cards are spliced into the existing MCNP deck, and any cards made obsolete by the change are removed. There are no persistent objects, and all macros inputs and outputs are displayed in labeled worksheet cells with in-situ documentation.

Typical workflow is shown in Figure 2. The loop model generator is provided with the endpoints of the desired timestep and a full-core MCNP deck for the starting time, complete except for dummy cells at loop sites. Once MCNP has returned tally results, the same spreadsheet calculates the burnup of all loop bundles according to equation (3).

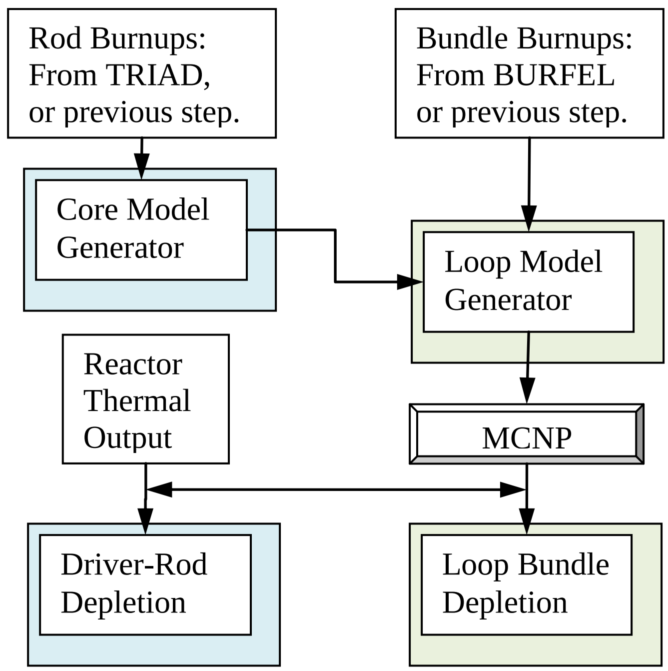

Figure 2 Workflow for a single timestep

In the present work, loop-string bundles have 36 pins arranged in concentric rings of 6, 12, and 18 pins. The center pin site is hollow, containing coolant and an Inconel tie rod. Individual pin composition and irradiation histories can vary within each ring, either due to a special test design, or due to the exchange of remountable pins. To account for all possibilities, pin-burnup is tracked individually, with the option to group pins together for tally purposes[3]. A model for 42-pin bundles was also implemented, and a model for 30-pin Material Test Bundles can be easily created.

The fuel-stack height is 48.2cm, divided into thirds for easy comparison with historical burnup-tracking methods. In addition, the top and bottom centimeter from the fuel stack are subdivided as distinct cells to better track end flux peaking effects. At the end of each fuel stack is a small air gap, within the sheath. The end-cap is modeled as a cylinder with radius matching the outer

[3] In the example discussed below, pins are grouped as “inner”, “inter” or “outer”, but this is not required.

radius of the fuel sheath. The heights of the air gap and end-cap are chosen so that the volumes of air, Zircaloy and coolant within the end region are conserved.

The typical 36-pin loop-string bundle is modeled using 180 fissile cells, and approximately 190 non-fissile cells including sheath coolant and the surrounding section of pressure tube. 42-pin models use 515 cells per bundle. Insertion of a single loop-string into the model implies the insertion of at least 2000 new cells and 1000 distinct material cards, though in practice many of the material cards are identical. A single loop string increases the overall complexity of the core model by roughly two thirds. Standard operation of the U2 loop involves two simultaneous irradiations, in which case non-loop cells, which represent almost the entire fissionable content of the NRU core, account for less than half the MCNP cells.

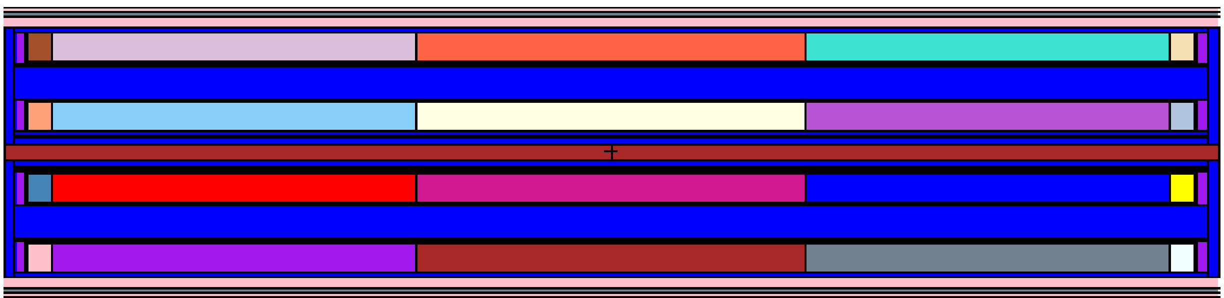

Figure 3 Axial cross section of a typical 36 pin loop-string bundle.

5. Preliminary Results

An irradiation of commercial-grade natural uranium bundles conducted over 13 days in November 2008 was simulated as a preliminary result. Net thermal output of NRU over this period was 1330 MWd. There were 27 driver rod and Mo-99 production rod movements during this period. BURFEL analyzed this irradiation in two timesteps, using six flux solutions from TRIAD3 simulations.

MCNP model convergence was tested by running 12 simulations with different random seed and source points. F7:n tallies of all cells agreed in all cases within ±1%. Runtime was approximately 125 cpu-hours for 1250 cycles of 100,000 histories; however wall clock time was longer when simulations were executed in parallel due to thread-synchronization between cycles. A trial simulation including photon production and transport took approximately 255 cpu-hours.

5.1 Snapshot Result

At the beginning of the irradiation period, the burnup of fuels in the core were copied from the measured burnups as reported by TRIAD3 (for driver rods) and BURFEL (for the loop site). Measured burnup is in units of measured channel thermal output per unit of fuel.. TRIAD3 is a self-consistent and validated neutronics diffusion code that normalizes burnup to the core power distribution [8]. To estimate the order of magnitude of uncertainty in the burnup, Figure 4 shows a comparison of the validated measured TRIAD3 results against a second parallel calculation by the same technique, but normalized only against overall reactor output. Overall there is very good agreement, as seen in Figure 4. TRIAD3 burnup values for the core loading in question appear uniformly accurate within ± 10 MWd per driver rod.

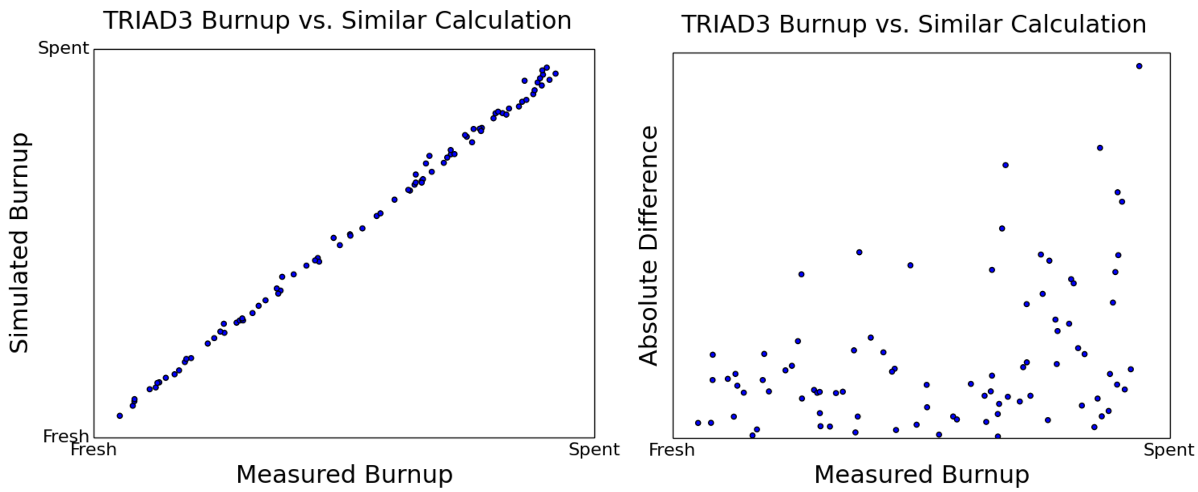

Figure 4 Comparison of TRIAD3 burnup versus a similar calculation, as a crude indication of burnup uncertainty.

To examine the sensitivity of the MCNP model to initial conditions, five trials of the same model were run. For each trial, the burnup of the 90 driver rods was randomly changed in order to roughly mimic Figure 4. Figure 5 shows the change in site F7 tallies, as a proportion of the total F7 tally of the appropriate trial, versus the chosen change in driver-rod burnup. Figure 5 suggests that the uncertainty in MCNP simulated driver rod power due to assumed uncertainty of the input burnup is on the order ± 1 kW, nine times out of ten.

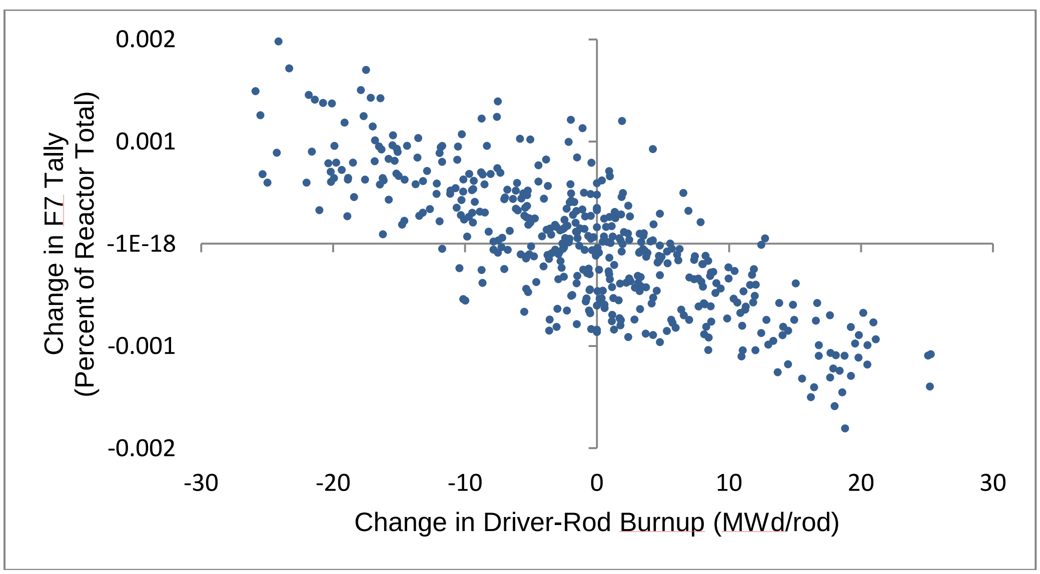

Figure 5 Change in site F7 tally versus perturbation of driver-rod burnup. 450 data points from 5 randomized trials.

Finally, the QFISS patch was used to adjust fission q-values to match WIMS-AECL total recoverable q-values, as outlined in Table 1. Figure 6 shows a comparison of the normalized F7:n tally conducted WIMS-AECL q-values versus the same tallies conducted using the default MCNP prompt fission q-values. The difference is comparable with the individual cell MCNP uncertainty, as simulated. The greatest differences align with the Mo-99 rod sites. Since the fissile content of Mo-99 rods is relatively small, the MCNP simulation uncertainty of tallies over these sites may be greater than expected. For this particular core loading, the difference in q-values does not appear significant to the loop site, L08.

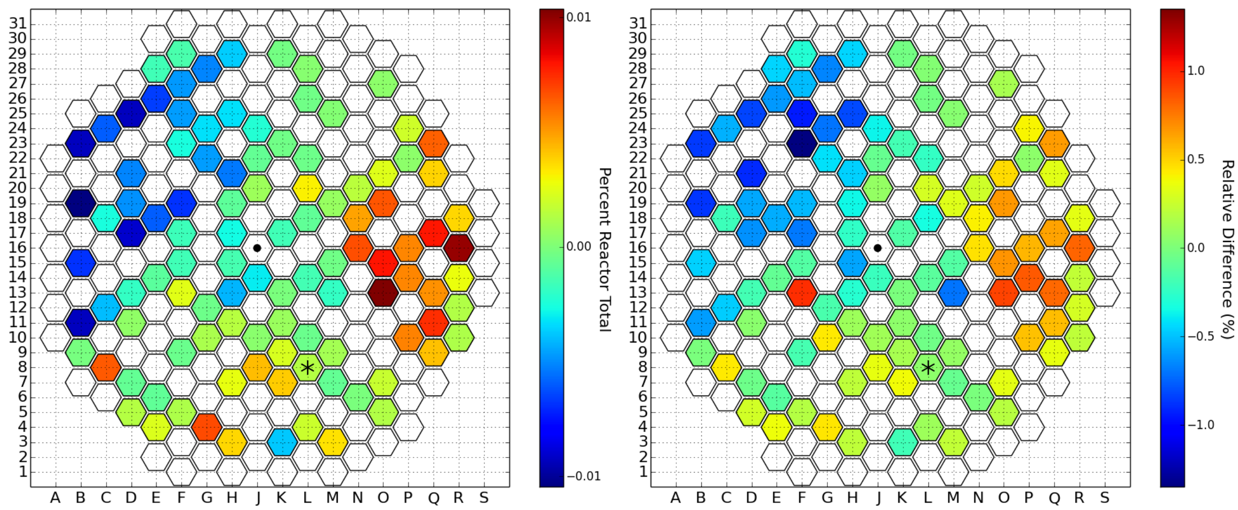

Figure 6 Comparison of normalized F7:n tally with WIMS-AECL q-values versus MCNP default prompt fission q-values (Table 1), in absolute and relative terms.

5.2 Burnup Result

To demonstrate the burnup capability of the spreadsheet macros, a series of five sequential simulations were conducted with the burnup of each loop bundle updated over each time period according to equation (2), above. The length of time periods were taken to correspond to intervals between TRIAD3 flux updates.

Figure 7 shows the result of this preliminary calculation in comparison with the result from BURFEL, in units of burnup per linear centimeter, normalized against total recorded burnup and displayed by segment. As discussed in section 4, there are five axial segments. Results from MCNP indicate end flux peaking in the final 1cm segments of the order of 20%, which is the magnitude to be expected [3]. MCNP also shows a slight downward flux tilt, which is not unexpected in a highly heterogeneous reactor.

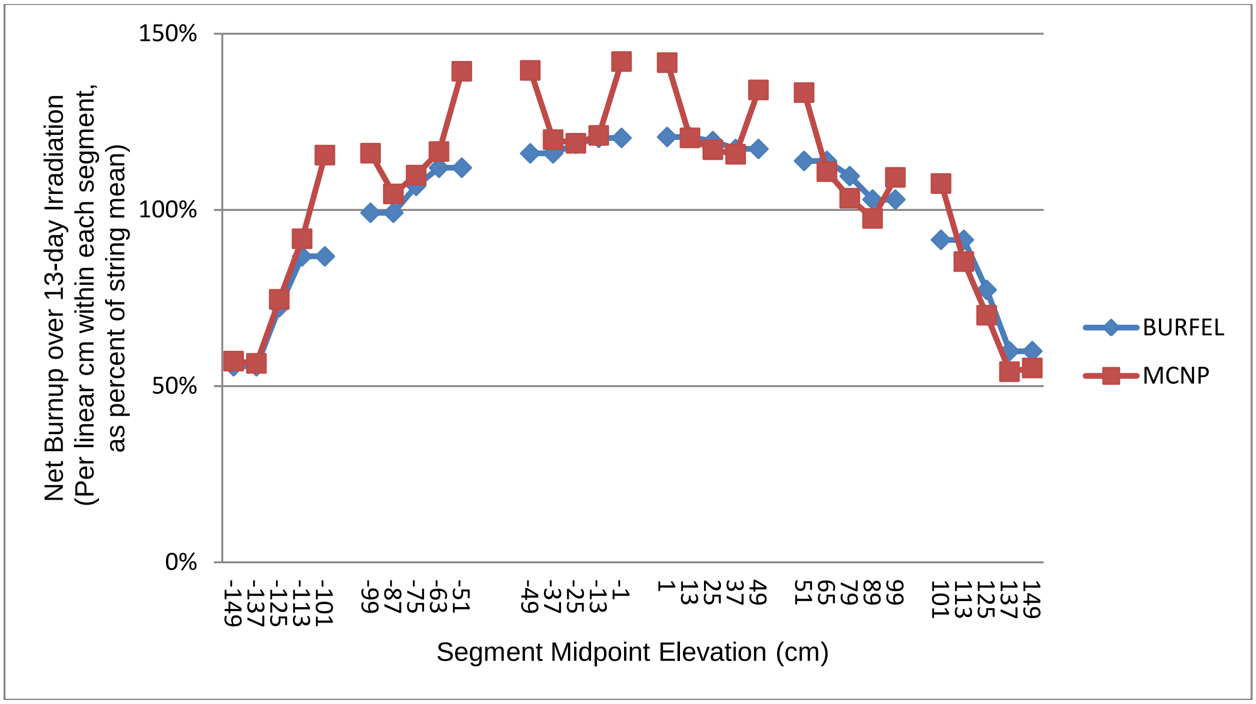

Figure 7 Loop site axial burnup under MCNP model versus as calculated by BURFEL.

6. Conclusions

A practical means to automatically extend the existing NRU full-core MCNP model to include loop strings has been created and tested. These extended models are necessarily complex. From a limited set of trials, reasonable model convergence appears to occur with only 125 million histories, and around 125 cpu-hours. The sensitivity of the model was examined through a limited set of randomized trials. On the basis of these trials, the initial data does not appear to be a concern. Adjustment of q-values used for tallying were made to compare the distribution of fission energy as normally tabulated by MCNP with the same distribution as it might be tabulated by WIMS-AECL. Differences observed were on the same order as the individual cell tally uncertainties. It was demonstrated that a burnup calculation may be conducted for the loop sites from intrinsic MCNP tallies. The axial flux profile from the MCNP model at the loop site over a 13 day irradiation showed expected end flux peaking effects, and generally matched historic predictions.

Insensitivity of the MCNP full-core NRU model to initial data should be properly quantified. Simulations with more histories and longer cycles should be conducted to ensure proper convergence. Due to model complexity, there is a risk of unintended importance sampling in neutron phase space due to the limited number of histories per cycle. An extension of the methodology described here to build a custom WIMS-AECL fuel table for each timestep should be considered. To verify the MCNP full-core NRU model, high-fidelity flux tallies should be conducted and compared to validated in-situ measurements.

The model described here is a successful proof of concept, and points the way toward more accurate prediction of loop fuel burnup, both to better understand the large record of historic irradiation data, and to better serve future customers.

7. References

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