Monte Carlo Calculations of Heat Deposition in Fuel and Non-Fuel Materials Irradiated in the National Research Universal Reactor (NRU)

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Abstract

Traditional reactor codes relate heat deposition in fuel and coolant to the fission power using approximate conversion factors, whose inaccuracy may lead to incorrect results that challenge the operating and safety limits imposed on channel power to coolant and/or heat ratings of fuel elements. The Monte Carlo transport code MCNP can be used for determining the heating power to fission power ratios (HPFPR) and power to coolant ratios (PTCR) for various types of fuel irradiated in NRU, depending on the fuel burnup. The method also applies to heating calculations of materials that contain no fuel. In-house patches to MCNP, QFISS (Fission Q-Values) and DPERT (Direct Cross-Section Perturbation), are incorporated for facilitating the process and dealing better with delayed energy deposition. As a result, this approach provides greater confidence that NRU remains within the license envelope.

1. Introduction

The NRU reactor at the Chalk River Laboratories is a heavy water cooled and moderated reactor, whose relatively large core consists of many different types of rods, such as driver fuel rods, Mo-99 production rods, test loops (each may be loaded with a string of different fuel bundles), other irradiation facilities and various absorber rods. Rods required to be cooled while the reactor is on power are usually installed in flow tubes, each with its own instrumentation for monitoring the coolant flow rate and temperature rise.

There are operating and safety limits imposed by the NRU Facility Authorization on the reactor thermal power, fuel channel power to coolant (PTC), element linear ratings and even heating of irradiation targets, as well as on fuel burnup. Of these, only the reactor thermal power and fuel channel PTC can be measured (based on the calorimetric data) and monitored in real time, but the others have to be evaluated off-line using computer codes such as TRIAD [1] (the NRU reactor finite-difference diffusion code) and BURFEL [2] (Burnup of Fuel Element – a system of codes and database for loop fuel calculations). These codes use various pre-computed neutronic data as functions of the fuel burnup whose inaccuracy may not only lead to incorrect results that challenge some of the above limits at a given time, but also accumulate to further affect future results.

To calculate fuel burnup and heat ratings, the measured PTC of a channel, based on its measured flow rate and temperature rise, is first converted to the fission power using a corresponding conversion factor, customarily known as the power to coolant ratio (PTCR). An increment of burnup for the whole rod in question is then calculated (to the accuracy of the measured data and

the PTCR used) and accumulated as the rod 'measured' burnup. TRIAD distributes the fission power and burnup axially over the rod length after a flux solution, using cell parameters which are functions of burnup. BURFEL distributes fission power and burnup both radially (from element to element in each bundle) and axially (over each element length), also using element linear burnups. Finally, the element linear rating at any given axial location is the linear fission power times the heating power to fission power ratio (HPFPR).

Discrepancies between the BURFEL and measured burnups in a number of irradiated loop fuel elements prompted a need to improve PTCR and HPFPR to be used in BURFEL. The MCNP (Monte Carlo N-Particle [3]) method has therefore been used for calculating these heat deposition ratios, which turn out to vary not only between fuel types but also with fuel burnup of a given type. In addition, MCNP can provide heating in non-fuel materials, mostly due to gammas.

Although MCNP itself can be used in principle to replace both TRIAD and BURFEL for providing all necessary neutronic and energy data in NRU, it is prohibitively costly and too slow to support NRU daily operations, and lacks burnup capability. Instead, it can be used to calculate the heating ratios and supply them as a function of burnup to the existing codes.

This paper presents results from MCNP calculations of the heating ratios for various fuel types and non-fuel materials. Material compositions as a function of burnup are taken from the WIMS [4] calculation used for preparing TRIAD or BURFEL neutronic data. Typically, the heating deposition ratios vary smoothly and slowly over a wide range of fuel burnup, and thus can be calculated at a few strategic intervals for the fuel lifetime and fitted by low-order polynomials.

2. MCNP calculations of heat deposition

2.1 Loop fuels

Various types of fuels (*e.g.*, containing natural uranium, slightly-enriched uranium, depleted uranium, plutonium, thorium, neutron absorbers, etc. including mixed fuel types) have been irradiated in the NRU loops, which are cooled by pressurized, high-temperature light water. A string of six modified-CANDU bundles[1] of different types and burnups may be installed in a loop test section. The PTCR concept is applied to a whole bundle at a given axial location, while HPFPR is applied to individual elements in the bundle. For each type of fuel bundle, a 2D MCNP model similar to its WIMS counterpart [2] is used for the calculation at a number of burnup intervals. At each step, the fuel material compositions in all elements for the MCNP calculation are taken from the WIMS results, corresponding to the axial element burnup. The criticality calculation mode (KCODE) is used in MCNP, with both neutron and photon capabilities. The output includes the fission (f_{mi}) and capture (c_{mj}) rates in any specified isotope (MCNP output Table 140), as well as both neutron and photon heating tallies (*F*6:*n* and *F*6:*p*) in every material (*m*) contained inside the pressure tube.

[1] Each bundle has the centre element removed for a tie-rod, and the remaining 36 (or 42) elements positioned in three rings – inner, intermediate and outer of 6, 12 and 18 elements, respectively (or 7, 14 and 21). Element locations are numbered counter-clockwise from the outer ring (*e.g.*, 1 or Outer#01) to the inner ring (*e.g.*, 36 or Inner#36).

MCNP tally *F*7:*n* provides the fission energy but includes only prompt terms of the total recoverable fission energy. The fission energy released by each fissionable isotope is customarily defined as that calculated in WIMS – the fission rate times the recoverable energy per fission (q-value), which also includes the delayed terms and excess neutron absorption term, in addition to that of MCNP. Table 1 lists the q-values from WIMS and MCNP for fissionable isotopes that may be present in NRU and loop fuels.

Table 1
Energy Release per Fission

Fissionable Isotope	Fission q-value (q_f MeV/fission)		
	WIMS ENDF/B-VI	WIMS ENDF/B-VII	MCNP5 (Table 98)
Th-232	191.613	195.570	171.91
U-233	200.005	200.308	180.84
U-234	197.590	200.383	179.45
U-235	202.356	202.382	180.88
U-236	202.346	203.037	179.50
U-238	204.489	207.205	181.31
Np-237	202.346	206.580	183.67
Pu-238	202.346	209.137	186.65
Pu-239	211.261	210.487	189.44
Pu-240	207.571	210.687	186.36
Pu-241	213.700	213.930	188.99
Pu-242	209.613	212.855	185.98
Am-241	214.489	214.850	190.83
Am-243	214.600	217.612	190.25
Cm-242	191.613	217.676	190.49

The fission energy (or power), *FP*, in each material *m* in the model is calculated as

$$FP(m) = \sum_i \left(f_{mi} \times q_{fi}\right) \quad (1)$$

where f_{mi} – the fission rate in isotope *i* in material *m*
q_{fi} – the WIMS fission q-value per fission event in isotope *i* (see Table 1)

Tallies *F*6:*n* and *F*6:*p* provide, respectively, neutron and gamma heating of a material but they lack any delayed terms that result from decays of fission and activation products. The delayed heating terms can be approximated by the total energy released from decays of fission or activation products, and any subsequent daughters, following a fission or capture event. Generally, the decay energy consists of: i) that being deposited locally (such as from beta or alpha particles, referred to as the delayed beta energy); and ii) that carried by emitted gammas which are transported and deposited elsewhere.

The total heating, *HP*, including the delayed energy depositions, of material *m* is calculated as

$HP(m) = HP{:}n(m) + HP{:}p(m)$, where (1)

$$HP{:}n(m) = F6{:}n(m) + \sum_i \left(f_{mi} \times q_{f\beta i}\right) + \sum_j \left(c_{mj} \times q_{c\beta j}\right) \quad (3)$$

$$HP{:}p(m) = F6{:}p(m) + \frac{F6{:}p(m)}{\sum_k F6{:}p(k)} \left[\sum_i \left(f_{mi} \times q_{f\gamma i}\right) + \sum_j \left(c_{mj} \times q_{c\gamma j}\right)\right] \quad (4)$$

where c_{mj} – the radiative capture rate in isotope *j* in material *m*

$q_{f\beta i}$, $q_{f\gamma i}$ – the average beta and gamma energy release from decay of fission products created from a fission event of isotope *i* (see Table 2)

$q_{c\beta i}$, $q_{c\gamma i}$ – the average beta and gamma energy release from decay of activation products created from a radiative capture in isotope *j* (see Table 3)

$\frac{F6{:}p(m)}{\sum_k F6{:}p(k)}$ – the mapping factor, the fraction of total photon energy deposited in material *m* (*i.e.*, the photon energy tally in a given material, *m*, to the sum of photon energy tallies over all materials in the model); *k* – the material index including *m*

Finally, the PTCR of a fuel bundle axial section is

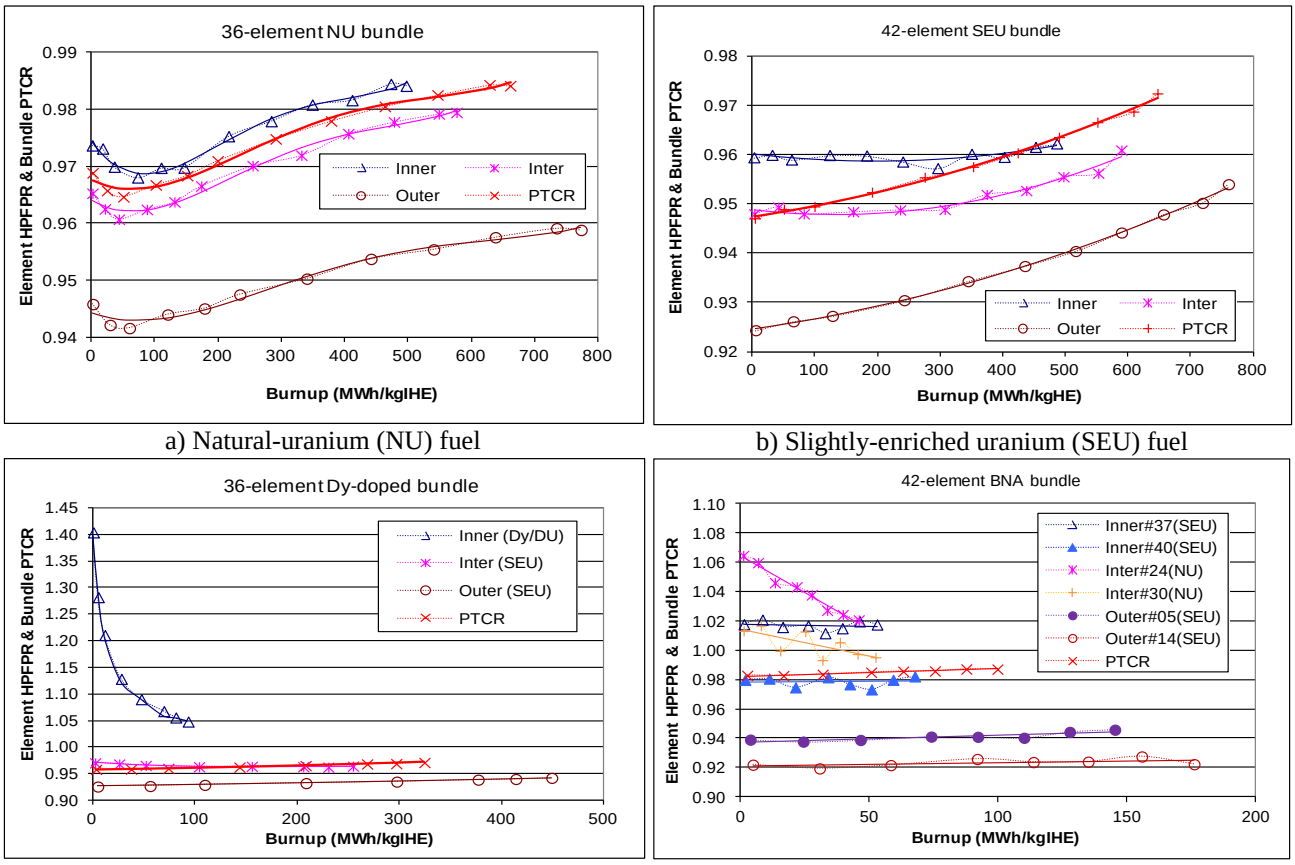
$$PTCR = \sum_m HP(m) \Big/ \sum_m FP(m) \quad (5)$$

and the HPFPR of a fuel element, m_f, (a material containing fuel) is

$$HPFPR(m_f) = \frac{HP(m_f)}{FP(m_f)} \quad (6)$$

For every fuel bundle, this process is repeated at a number of burnup steps with only the compositions of burnable materials changed to correspond to the burnup step.

Figure 1 presents the element HPFPR and bundle PTCR for several loop fuel bundles vs burnup (MWh/kgIHE – Initial Heavy Element). Generally, the bundle PTCR, ranging from 0.945 to 0.985, increases with fuel burnup, except for natural uranium fuel having burnup below ~100 MWh/kgIHE (in which Pu-239 is still building up). Bundles containing more highly enriched fuel and less absorber have a smaller PTCR. Element HPFPRs vary not only with burnup but also strongly from ring to ring in a bundle. Like the bundle PTCR, an element HPFPR also increases with burnup, except for initial-burnup NU fuel and those containing absorbers. It is interesting to note that elements containing strong neutron absorbers may have an HPFPR greater than 1.0 since they normally have a low fission power but a relatively large heating power due to gammas emitted from neutron captures in the absorbers as well as from decays of the resulting activation products. The gammas from absorber elements also affect the heating of nearby elements, resulting in quite different HPFPR's in fuel elements of the same type but located near to or far away from the absorber element (Figure 1 d).



a) Natural-uranium (NU) fuel

b) Slightly-enriched uranium (SEU) fuel

c) Dy-doped depleted-uranium (Dy/DU) fuel

d) Fuel near burnable neutron absorbers (BNA)

Figure 1 Examples of heat deposition data in loop fuel bundles

2.2 QFISS and DPERT patches

To implement the method described above, a great amount of MCNP output data - the fission and capture rates in every nuclide in all materials of the model - was required to be put into a spreadsheet for manual processing, a process prone to errors. Also, the delayed gamma energy deposition was distributed proportionally to the *prompt* gamma energy deposition, as in equation 4 (aka *photon mapping*), without tracking explicitly the transportation of these delayed gammas. Two in-house MCNP patches, QFISS and DPERT, were developed and can be incorporated at the execution time to overcome these problems.

QFISS replaces the MCNP hard-wired prompt q-fission values (Table 98) with those customarily used in reactor physics codes (*e.g.*, WIMS total recoverable q-fission values in Table 1). As such, MCNP fission tally *F*7:*n* will be equivalent to the fission power calculated by these codes, *i.e.*,

$$FP(m) = F7{:}n(m) \qquad (7)$$

Table 2
Delayed energy data for fission

(n, f)	Total delayed beta energy ($q_{f\beta}$ MeV/fission)*	Total delayed gamma energy ($q_{f\gamma}$ MeV/fission)*	Average prompt gamma energy ($E_{fp\ ave}$ MeV/γ)**	Delayed γ's $\gamma_d = q_\gamma / E_{p\ ave}$
Th-232	8.38	8.16	0.94803	8.61
U-233	5.16	5.01	0.86653	5.78
U-234	6.25	6.13	0.88671	6.91
U-235	6.50	6.33	0.93767	6.75
U-236	7.56	7.42	0.88679	8.37
U-238	8.48	8.25	0.88689	9.30
Np-237	6.41	6.28	0.93847	6.69
Pu-239	5.31	5.17	0.87041	5.94
Pu-240	6.62	6.49	0.86596	7.49
Pu-241	6.58	6.40	0.88711	7.21
Pu-242	7.87	7.72	0.86891	8.88
Am-241	5.62	5.51	0.87616	6.29
Am-243	6.75	6.62	0.88533	7.48
Cm-242	5.64	5.49	0.88512	6.20

(*) ENDF/B-VII neutron data (*http://t2.lanl.gov/data/neutron7.html*).

(**) $E_{fp\ ave}$ – the average energy of the prompt gammas emitted from fission, calculated with Watt's thermal-induced U-235 fission neutrons, using the ENDF/B-VII neutron cross-section library.

Table 3
Delayed energy data for neutron capture

(n, γ)	Total delayed beta energy ($q_{c\beta}$ MeV/fission)*	Total delayed gamma energy ($q_{c\gamma}$ MeV/fission)*	Average prompt gamma energy ($E_{p\ ave}$ MeV/γ)**	Delayed γ's $\gamma_d = q_\gamma / E_{p\ ave}$
Th-232	0.624	0.260	4.7864	0.054
U-236	0.184	0.143	5.1259	0.028
U-238	0.65	0.235	4.8063	0.049
Np-237	0.211	0.581	5.4881	0.106
Pu-242	0.169	0.025	5.0345	0.005
Al-27(1)	1.242	1.779	> 3.802	0.0068
Mn-55(1)	0.831	1.691	> 2.669	0.0048
Co-59	0.15	2.51	3.0578	0.821
Zr-94	0.12	0.733	2.1076	0.348
Y-89	0.98	0.634	2.2907	0.277
Gd-158	0.31	0.052	1.8618	0.028
Gd-160	0.583	0.388	1.7278	0.225
Dy-164	0.546	0.046	1.6216	0.028
Ir-191	0.267	0.818	1.627	0.503
Ir-193	0.888	0.867	1.76	0.081
Te-126	0.31	0.02	n/a	No photon production data
Te-128	0.6	0.01	n/a	
Te-130	1.2	2.2	n/a	

(*) ENDF/B-VII neutron data (*http://t2.lanl.gov/data/neutron7.html*).

(**) $E_{p\ ave}$ – the average energy of the prompt gammas emitted from capture, taken from output Table 140 for NRU.

(1) Except for Al-27 and Mn-55, these γ_d values add the correct amount of energy.

DPERT, on the other hand, adds the delayed energy from decay of fission or activation products. The delayed beta energy ($q_{f\beta}$ or $q_{c\beta}$) is added directly to the reaction q-value, fully deposited locally and recorded in MCNP neutron heating tally *F*6:*n*. Addition of the delayed gamma energy, however, is not straightforward, and is added as additional equivalent prompt gammas carrying the correct amount of energy. Knowing the average energy of prompt gammas ($E_{p\ ave}$, MeV/γ) emitted from a fission or activation reaction and the delayed gamma energy ($q_{f\gamma}$ or $q_{c\gamma}$, MeV) from decay of the resulting fission or activation products, the number of such 'delayed' gammas is

$$\gamma_d = q_\gamma / E_{p\ ave} \quad (8)$$

The delayed gammas are transported and deposit their energy over the model in a realistic manner, rather than being forced to follow the global prompt gammas distribution by the photon mapping technique. As a result, the MCNP photon heating tally *F*6:*p* will fully account for the deposition of the delayed gammas. The total heating of material *m* is computed by MCNP as

$$HP(m) = F6{:}n(m) + F6{:}p(m), \text{ the same as } F6{:}n,p(m) \quad (9)$$

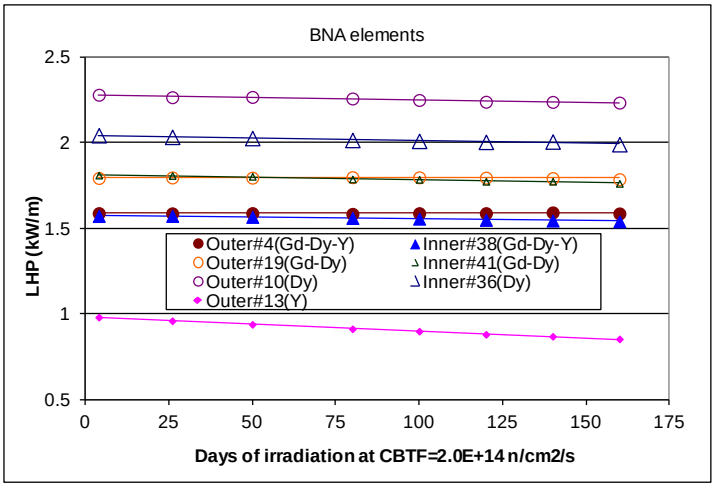
Note that the cross section libraries for some nuclides (*e.g.*, all tellurium isotopes) lack photon production data and cannot be supported by DPERT. Also, for some nuclides such as Al-27 and Mn-55, due to the complexity of photon production data in their libraries, appropriate values of γ_d have to be manually evaluated on a case-by-case basis.

It should be stressed that DPERT is designed to be used only for energy deposition calculations, and is unlikely to be valid for cases sensitive to gamma spectrum. The reason is that DPERT produces the delayed gammas with the prompt gamma spectrum, which is generally far harder than is the delayed spectrum. Since the majority of delayed gammas are eventually absorbed within the reactor core environment, their spectrum is of little significance when applied only to energy deposition.

2.3 Non-fuel materials

Materials that contain no fuel do not involve fission powers or burnups but do involve heating powers, so the HPFPR concept generally does not apply to them. Non-fuel element heating powers are directly obtained from the MCNP tally *F*6:*n,p*, normalized to a specific operating condition.

Figure 2 presents linear heating powers (LHP) in the burnable neutron absorber (BNA) elements installed in a loop fuel bundle, whose PTCR and fuel-element HPFPR's are illustrated in Figure 1 d), at a loop cell boundary thermal flux (CBTF) of 2.0E+14 n/cm^2/s. It is necessary for BURFEL to also produce LHP in BNA elements together with fuels irradiated in the loop under the actual operating conditions. The HPFPR parameter can be used to 'carry' the LHP value to BURFEL. To accomplish this, BNA elements are given fictitious fission power ratings (LFP) *invariant with burnup* (*e.g.*, 0.1 kW/m); their HPFPR values are then the LHP from MCNP divided by that fictitious LFP (*e.g.*, 10 times LHP). To track the irradiation time for BNA elements, they are also given a fictitious burnup equivalent to the CBTF fluence (*e.g.*, days of CBTF=2.0E+14 n/cm^2/s). As such, BURFEL will treat BNA elements as if they were fuel.



BNA – burnable neutron absorber, a blend of oxides of Zr and any of Gd, Dy or Y
CBTF – cell boundary thermal flux, an average thermal flux level at the loop site boundary

Figure 2 Heating of BNA elements in a loop bundle

There may be more effort required when dealing with materials containing nuclides whose cross section libraries lack photon production data. The following example calculates the heat loads, corresponding to the operating limit, in capsules containing iridium and tellurium targets installed in a six-barrel multi-capsule rod (MCR6) in NRU. A straightforward application of the method would give ~150 W/Ir-capsule, and ~300 W/Te-capsule, which is obviously incorrect (natural iridium is a very much stronger neutron absorber than natural tellurium). The reason is that the library used for tellurium isotopes does not include the photon production data, resulting in a completely local deposition of all neutron-Te reaction energy release. This leads to a great overestimation of heating in Te-capsules and an underestimation of that in Ir-capsules (due to the missing gammas from Te-captures).

Table 4
MCR6 capsule heat load

Capsule	Prompt neutrons	Te-capture gammas	Prompt gammas	Delayed gammas	Delayed betas	Total (W/capsule)
Ir	0	6 (3%)	93	20	40	**158**
Te	(201)	27 (13%)	66	17	7	**117**

By performing MCNP calculations twice, one with DPERT and the other without DPERT, for the same MCR6 model containing the two types of capsules, heating components in each capsule can be obtained, as shown in Table 4. It shows that ~200 W in a Te-capsule was from the capture of neutrons (*F*6:*n*), and this energy should be carried away by gammas, similar to those from Ir-captures. To redistribute the Te-capture energy properly requires an additional calculation with the only gamma source being a gamma spectrum from Te-123 captures (Te-123 has an abundance of only 0.89% but contributes ~90% of all neutron captures in natural tellurium). The mapping technique (with mapping factors as in equation 4) was then used to find that, with proper gamma transportation, the majority of the Te-capture energy (*i.e.*, 200 W/Te-capsule)

actually heated the coolant and other materials, while only 13% was deposited in the Te-capsules and 3% went into nearby Ir-capsules. As a result, more realistic heat loads of 160 W/Ir-capsule and 120 W/Te-capsule were found, well below the prescribed limits.

2.4 Full core calculation

Powers to coolant (PTC) in NRU are monitored and used for calculating assembly measured burnups, customarily defined as the accumulated *fission* energy in a unit of fuel (MWd/rod, or MWd/cm). Rod burnups are calculated from the energy to coolant integrated over time and PTCR (currently used values in TRIAD are 0.94 for driver fuel rods, 0.88 for Mo-99 production rods, 0.96 for fuel-loaded loops). However, as exemplified in Figure 1, PTCR values can vary considerably, depending on fuel type and burnup.

It is possible to use an MCNP full-reactor model [5] to calculate heating rates for all NRU sites at once, including the driver fuel rods of various burnups ranging from fresh to the exit burnup. Fission powers are tallied by *F*7:*n* and heating powers by *F*6:*n*,*p*. In particular, heating in each fuel channel can be tallied separately for outside of flow tube (the moderator) and inside, equivalent to the channel PTC. The channel PTCR is then the ratio of *F*6:*n*,*p* inside the flow tube to its *F*7:*n*. The total *F*7:*n* is the reactor fission power.

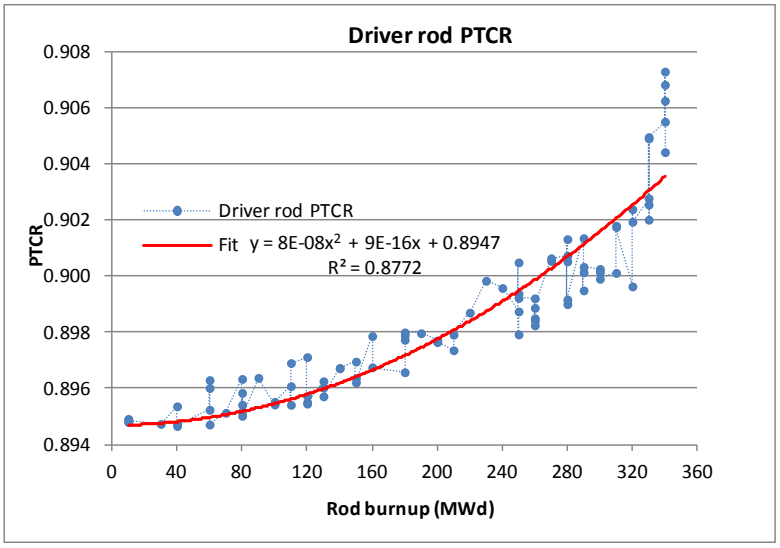


Figure 3 NRU driver rod PTCR vs burnup

Figure 3 shows the PTCR in NRU driver rods increases slightly with the rod burnup, averaging around 0.9. Table 5 provides a summary of the reactor power data, normalized to a reactor fission power of 100 MW, for a typical operating core.

Table 5
NRU core heating calculation

Category	Number of sites	Fission (MW)	Site heating (MW)	PTC (MW)	Average PTCR
Core (excluding loop)	-	**100.0**	**99.1** (reactor thermal power)	-	-
Driver fuel rods	90	96.45	91.42	86.59	0.895
Mo-99 rods	15	3.55	3.84	3.28	0.925
Loaded loop (fresh NU bundles)	1	2.74	2.71	2.64	0.963
Non-fuel sites	121	0	3.80	-	-

Note that the loop fuel PTCR from this 3D calculation is consistent with that from a simple 2D model (Figure 1 a), which is more efficient to use. Also, ~99% of the reactor fission power is taken out by the cooling system, known as the reactor thermal power (excluding heating due to coolant frictions and heat loss to the ambient environment in the primary cooling system), and less than 1% is deposited in the outer structure of NRU.

3. Conclusions

The MCNP method, patched with QFISS and DPERT, has been used for calculating heat deposition in fuel and non-fuel materials irradiated in NRU. The fuel PTCR and HPFPR values vary depending on fuel type and burnup. The MCNP method produces more reliable estimates of heating power ratios than the previous estimates, which results in less uncertainty in power-related safety-significant parameters. This in turn provides greater confidence that NRU operation remains within the license envelope.

4. References

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