### VALIDATION OF THE TRIAD3 CODE USED FOR THE NEUTRONIC SIMULATION OF THE NRU REACTOR

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#### Abstract

The neutronic simulation of the NRU research reactor at Chalk River is performed by the TRIAD3 code. TRIAD3 is a three-dimensional code using a modified neutron diffusion theory in two-energy groups. The modification is the use of <u>cell discontinuity factors</u> (*cdf*) to improve the radial neutron leakage calculation between adjacent cells. This paper describes three validation exercises performed over the past few years. It describes methods of obtaining the flux, power and reactivity measurements from the NRU reactor and presents comparisons between these measurement data and code simulation results.

## 1. Introduction

The Nuclear Research Universal (NRU) reactor at Chalk River began operation in 1957. It is used to carry out research in basic science and in support of the CANDU power reactor program. It is also a major supplier of medical radioisotopes in Canada and the world. The NRU reactor is heavy water cooled and moderated, with on-line refueling capability. It is licensed to operate at a maximum power of 135 MW, and has a peak thermal flux of approximately  $4.0 \times 10^{18} \text{ n.m}^2 \text{.s}^{-1}$  [1]. Figure 1 shows an NRU core lattice, with 31 rows and 18 columns (A to S, with no column "I"). The hexagonal lattice pitch between adjacent sites is 19.685 cm.

Neutronic simulation of the NRU reactor is performed by the TRIAD3 code [2]. Operational data on flux, power and reactivity measurements are also available, and these data were collected and analyzed, and compared with the simulation predictions to validate the TRIAD3 code. This paper describes three validation exercises that were performed in the past few years. It describes methods of obtaining measured data, and presents comparisons between the measured data and simulation results.

# 2. Overview of the TRIAD3 code

The TRIAD3 code was developed in the mid-1980s to perform various physics calculations for the NRU reactor, including core power calculations for determining burnup and depletion in the assemblies in the reactor, reactivity calculations for determining rod shuffles for on-power refueling, control rod worths, reactivity worth of



Figure 1. The NRU core lattice.

voiding the coolant in a loop, and fast neutron flux levels in material specimens inside fast neutron rods. In the present TRIAD3 code version, 301-rod sites are modelled. In the radial direction, each hexagonal cell is modelled as 6 triangular prisms. In the axial direction, a total of 18 planes, each of variable cell height to match the fuel lengths of the various rod types in the reactor, are used. There are a total of 6x301x18 triangular prisms (or meshes) for the whole reactor.

The NRU reactor consists of many different types of rods, such as driver fuel rods, fastneutron rods, Mo-99 production rods, loop fuel strings for advanced fuel bundle testing, absorber rods and control rods. The 18 axial cells representing a rod in NRU can be of different types, but each cell type has the same uniform neutronic properties. The detailed flux shapes and neutron spectrum through each type of cell are determined using the WIMS-AECL neutron transport code [3]. The homogenized cell parameters, in two energy groups, are then calculated by flux- and volume-weighting the region material properties. Examples of cell parameters are diffusion coefficients and various cross sections, such as absorption, removal and fission. After the cell parameters are calculated, the flux and power distributions for the cells in the NRU core can be determined using a modified neutron diffusion theory. The modification is the use of <u>cell discontinuity factors</u> (*cdf*) to improve the radial neutron leakage calculation between adjacent cells. The usual inter-cell leakage calculation in the finite-difference diffusion theory uses a simple linear model, which distorts the flux distribution except in relatively uniform reactors. Since the NRU reactor is made up of many different types of rods, some with very different neutronic properties, it is necessary to use *cdf* s in TRIAD3 to adjust the neutron current calculation at the homogeneous cell boundaries to minimize these distortions. The *cdf* is calculated from the ratio of the heterogeneous to homogeneous cell boundary flux. The heterogeneous cell boundary flux is determined from the WIMS-AECL flux shape by extrapolating the last 3 mesh point fluxes inside the boundary of the actual cell. The homogeneous cell boundary flux is determined from the boundary flux of a cell having the uniform homogenized cell parameters throughout the cell.

The lattice split of NRU between columns D and E, (as shown in Figure 1), is approximated geometrically by slabs located between the gaps of the triangular cells in each column. The neutronic effect of the lattice split is simulated by a response matrix which links together the surface fluxes and net currents of the neighbouring triangular cells on either side of the split, using also two group diffusion equations.

In the TRIAD3 code, the two-group diffusion equations in three dimensions are solved numerically using a finite difference method. The difference equations for the group fluxes in each triangular prism of an NRU hexagonal cell are solved using flux iteration techniques, and to accelerate the flux convergence process successive point over-relaxation is used. After the fluxes in all prisms are determined, the flux in a hexagonal cell is calculated from the average of the fluxes of the six triangular prisms for that cell. The power generated from a hexagonal cell is calculated from the product of the cell flux, the cell volume and the Q value, which is the linear heat rating per unit flux per unit cell volume.

# 3. Validation using flux measurements

### 3.1 Thermal neutron flux measurements

This validation exercise compared axial flux distribution predictions from the TRIAD3 code, with the corresponding measured distributions over a 4-year period between 2000 and 2003. The thermal neutron flux measurements were conducted in three monitoring sites P18, L06 and E22, adjacent to the loop fuel bundle testing sites. Each of the flux detector rods, in sites P18 and L06, contains six vanadium self-powered neutron flux detectors of the coiled type, while the flux detector rod at the E22 site contains nine operating vanadium detectors of the SIR (Straight Individually Replaceable) type. In TRIAD3, each monitoring site was modeled as an actual flux detector rod with a central hollow tube for the access of a Travelling Flux Detector for the purpose of periodic calibration of the stationary detectors. The vanadium detectors were initially calibrated

in a known thermal flux in the ZED-2 reactor at Chalk River, and later re-calibrated, insitu, by Traveling Flux Detector (TFD) scans, with the reactor operating at constant power. The currents from each detector were taken through a precision resistor to provide a voltage in the range of 0 to 50 millivolts for REDNET to monitor. REDNET, Reactor Data NETwork, is the data acquisition and processing system for the NRU reactor. The detector measurement error itself, including the burnup correction uncertainty was about  $\pm 3\%$ . However, no empirical correlation between the measurement error and the burnup of the detectors has been established for the past years.

## 3.2 Comparison of measured and simulated fluxes

Thermal neutron fluxes at detector locations were measured with different fuel strings in the adjacent loop fuel test sites, and on some occasions, with no fuel strings in the loop test sites. After the flux measurement data were corrected for burnup of vanadium, they were compared with the simulated fluxes. For normalization, the simulated fluxes determined by the TRIAD3 code are first normalized to 1.0 at the flux peak. The measured fluxes are then normalized to the simulated fluxes such that the sums of the squares of the differences between the measured and simulated fluxes. The normalization factor for the measured fluxes at the detector locations of the monitoring site,  $a_N$ , is

$$a_{N} = \sum_{i} (\phi^{*}_{sim,i})^{2} / \sum_{i} \phi^{*}_{sim,i} \times \phi_{mea,i} , i = 1, \dots, k$$
(1)

where  $\phi^*_{sim,i}$  is the normalized simulated fluxes at detector location, *i*,

 $\phi_{mea,i}$  is the measured fluxes at detector location, i, and

k is the number of detectors at the monitoring site.

The normalized measured flux at detector location, *i*, denoted by  $\phi^*_{mea,i}$ , is determined by

$$\phi^*_{mea,i} = a_N * \phi_{mea,i} \tag{2}$$

The comparison of the measured and simulated fluxes in sites P18 and L06 has been reported in the 28<sup>th</sup> CNS conference in 2007 [4]. An axial flux profile at site E22 on 2002 March 15, with fuel string S293 having an uniform natural uranium bundle loading in the adjacent loop fuel test site is shown in Figure 2. The flux distribution was symmetrical about the centre of the reactor. The difference between the measured and calculated fluxes at the bottom detector location was +5.7%, and at the rest of the detector locations the differences were better, within  $\pm 3.8\%$ .

In summary, from the flux measurement data covering over a 4-year period between 2000 and 2003, the TRIAD3 code was validated for predicting the relative axial flux shape within 6.5%. During this validation exercise, there were no loop strings that resulted in

flux depression in the axial central region of the reactor. The maximum measurement error for an individual detector for this period was  $\pm 4.5\%$ , but the average value taken over all detectors for a particular flux-monitoring site was  $\pm 3.0\%$ .



Distance from Centre of Reactor, cm

Figure 2. Comparison of axial measured-to-simulated fluxes on 2002 March 15 at Site E22.

# 4. Validation against power measurements

# 4.1 Power measurements and comparison with simulated powers

Power measurement data for the validation exercise covered three years from 2002 to 2004, at approximately equal intervals of ~7 full-power days (i.e., not counting the days for shutdown). The data were selected to cover the wide range of operational conditions normally encountered in NRU. The measured powers to the coolant at driver fuel and Mo-99 production sites are calculated from the scan data of the reactor, which consist of the heavy water coolant temperature rise and flow rate measurements, all taken at a specific date/time and TPD (Total Power Developed in units of MWd). The power to the coolant in MW,  $P_{C_i}$ , at a reactor site *i*, can be calculated from the scan data:

$$P_{C_i} = \Delta T_i * G_i * c \tag{3}$$

where  $\Delta T_i$  is the heavy water coolant temperature rise in °C,

 $G_i$  is the measured flow rate of the coolant, in IGPM, imperial gallons per minute, and

c is the specific heat of the heavy water coolant, taken to be 0.000347, in MW per (IGPM- $^{\circ}$ C).

The flow rate,  $G_i$ , is determined from a pressure measurement in a 'sample line'. For loop sites the method for calculating the measured power is similar, except that the coolant in the loop is light water and the value for the specific heat, c, in Equation (3) will be slightly different.



Figure 3. Histogram of the measured-to-simulated power ratios of fuel rods at Site C18.

The fission power of a fuel rod or loop fuel string based on measurement,  $P_{mea,i}$  can be determined from its power-to-coolant ratio by

$$P_{mea,i} = P_{C,i} / R_{PTC} \tag{4}$$

where  $R_{PTC}$  is a separately calculated or estimated power-to-coolant ratio to account for the fission energy not being absorbed by the coolant. There are sources of measurement

errors in both the temperature rise and flow rates. The errors were found to be fairly constant throughout the past years, and they were estimated to be about  $\pm 7\%$  (1  $\sigma$ ) each. Assuming that the temperature and flow measurements are not correlated, the combined error for the temperature rise and flow measurement is  $\pm \sqrt{(0.07)^2 + (0.07)^2} = 0.099$ , or about  $\pm 10\%$ .

In order to calculate the power ratios, both the measured and simulated power distributions were normalized to the same total reactor power of 100 MW. Power ratios for driver fuel rods, Mo-99 isotope production rods and loop fuel assemblies are calculated in NRU on a routine basis. Figure 3 shows a typical histogram of the

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**Note:** The underlined sites are the Mo-99 Production Rod sites. The bold italic sites are the loop fuel sites, and the rest are the NRU driver fuel rod sites.

Figure 4. Distribution of the averaged measured-to-simulated power ratios in NRU from 2002 to 2004.

measured-to-simulated power ratios of the fuel rods at site C18. In this Figure, a normal (Guassian) distribution based on the calculated mean value and standard deviation from the data is also shown in the background to compare with the actual frequency

distribution. For this site, the mean value for the power ratio is 1.013, and the standard deviation is  $\pm 0.056$ .

Figure 4 shows the distribution of the averaged measured-to-simulated power ratios over the 3-year period. Relative to measurements, it was found that TRIAD3 over-predicted the driver fuel rod power by 1.0 %, and the standard deviation for the measured-tosimulated power ratios was  $\pm 6.1\%$ . The Mo-99 production rod power was underpredicted by 14.1 %, with a standard deviation of  $\pm 9.3\%$ . For loop powers, the simulation results show less than 4.5% over-prediction for the loop fuel strings in the E20 and L08 loop sites, but 9.2 % under-prediction in the O17 loop site. The standard deviations in the measured-to-simulated power ratios for the loop fuel strings were below  $\pm 4.3$  %. In addition, there seems to be systematic variation in the measured-to-simulated power ratios in Figure 4: higher at the right side than at the left side, and at the top compared to the bottom. The variations are not random, and could be due to the inadequacy of the neutronic modeling at the irregular physical boundary of the NRU reactor and the sensitivity of the leakage fluxes at those locations. An example of the irregular physical boundary is the thermal column experimental facility on the east face of the reactor, measuring 2.4 m by 2.4 m.

The standard deviations for loops are smaller than for driver rods due to their better power monitoring systems, and in part due to their locations in the core. All the loop sites are located close to the "centroid" of the Bessel radial flux profile. For Mo-99 rods, the average power ratios are high. This may be due in part to approximations in the axial smearing within the TRIAD3 meshes, but is more likely due simply to the fact that these rods operate at low power compared to nearby driver rods, and thus the sample line probably picks up heat from the surroundings during transmission to the temperature sensor. Variation in heat pick-up, relative to the low rod power, would also explain the larger standard deviation for these rods.

# 5. Validation against reactivity measurements

# 5.1 Reactivity changes for fuel rod shuffles

Reactivity values for NRU core loading changes are calculated using TRIAD3. For driver fuel rod changes, which are done on-power, the operating control rod moves to compensate for the fuel rods being removed or inserted. Measurements of control rod positions from equilibrium conditions before and after a shuffle can be compared with the simulated reactivity worth of the whole shuffle. Usually in a whole shuffle, several fuel rods move from one site to the next, starting with a fresh rod and finishing by removing an old one. The error in reading the control rod position in the range of interest is small, less than 0.1 mk. This reactivity validation is not really a validation, as would be achieved from the transient measurement, such as rod drop experiments. Instead, it is an inter-comparison of reactivity values calculated by TRIAD3, and the reactivity changes from the control system are treated as measured reactivity values. The reactivity value of a control rod or a fuel rod is calculated by taking the difference of the (1/k-eff) values of two cores: one with the rod in, and the other with the same rod out. The calculated reactivity value of a rod is also sensitive to the burnup of its neighbouring rods.

Measured data for control rod (including adjuster rods) positions and reactor TPD values before and after rod shuffles were retrieved for a period from 2006 January to 2007 November. The data included a variety of fuel shuffles, from two-rod to five-rod shuffles, and covered different sites within the NRU reactor. One-rod shuffles were not considered because they occur rarely and usually induce severe flux tilts. In column 2 of Table 1, each shuffle involves at least 2 rods. For instance, "R14-> M07" stands for a shuffle in which a fresher rod was put into site R14, and the original rod at site R14 was moved to site M07. The control rod position and TPD value at the end of a shuffle were determined after most of the transient effects had died away and equilibrium condition was re-established. In collecting the data, this was assumed to be about two hours after the last rod of the shuffle had been put back into the reactor. The measured reactivity change for a shuffle was determined by taking the difference of the reactivity scale values associated with the before and after control rod positions.

The measured reactivity change was corrected for fuel burnup during the shuffle by adding a burnup correction factor, determined by multiplying the burnup reactivity coefficient (taken as 16.7 mk / 1000 MWd in this case) by the TPD difference for the shuffle. The burnup correction factor can be significant, as much as one mk, due to the length of time, often over half a day, needed to complete a four- or five-rod shuffle. In this validation exercise, the burnup refers to the fuel burnup for the whole reactor. For example, 100 MWd burnup refers to the energy generated by the fuel consumption of the reactor, operating at 100 MW for 1 day.

# 5.2 Comparison of measured and simulated reactivity changes

Comparisons of measured-to-simulated ratios for fuel shuffle reactivity changes over two years are presented in Table 1. The measured-to-simulated ratios show a random variation about a mean value. The average measured-to-simulated ratio for the reactivity changes of NRU driver fuel rod shuffles was 1.088, and the standard deviation was  $\pm 9.9\%$ .

For comparison with the expected uncertainty, it may be noted that reactivity is a function of flux and adjoint flux. The adjoint flux distribution is usually similar to the flux distribution, though often flatter, so the flux may be taken as a first approximation of the adjoint flux. The previous power validation exercise (Section 4) showed the TRIAD3 calculated power distribution (and therefore flux to a large degree) is precise to  $\pm 6.1\%$ ,  $1\sigma$ , and this would indicate that the precision of the reactivity calculation should be roughly  $2x \ 6.1\% = 12.2\%$ . This is consistent with the current analysis.

Date	Shuffle	Contro Posit Before S	l Rod ion Shuffle	Control Positi After Sl	l Rod ion huffle	"Measured" Reactivity Change (mk)	Burnu Correct	p ion	Total "Measured" Reactivity Change	TRIAD3 Fuel Shuffle Change	Mea-to- Sim Ratio			
		CR (position)	CR worth	CR (position)	CR worth	, , , , , , , , , , , , , , , , , , ,	TPD Before/after*	mk	mk	(mk)				
27-Jan-06	H29->L04 ->J20->F03	17(96)	10.3	16(182)	7.6	4.86	968776.2/ 968836.3	1.00	5.86	6.1	0.96			
18-Feb-06	J24->L1 ->E04	AR3(193)	8.2	AR3(125)	8.2	2.87	970636.8/ 970698.6	1.03	3.90	4.1	0.95			
19-Feb-06	R14->M07	17(212) AR3(100)	7.1 8.5	17(190) AR3(50)	7.1 8.5	1.44	970755.6/ 970779.8	0.40	1.84	1.8	1.02			
21-Feb-06	Q23->G28	17(194)	7.1	17(154)	7.1	1.42	970999.8/ 971023.5	0.40	1.82	1.8	1.01			
22-Feb-06	J14->M09 ->E28	17(220)	7.8	17(158)	7.8	2.57	971119.3/ 971195.8	1.28	3.85	4.2	0.92			
23-Feb-06	B19->F27 ->L14	17(196)	7.3	17(92)	7.3	2.56	971244.2/ 971293.5	0.82	3.38	3.1	1.09			
24-Feb-06	D21->P10	17(114)	7.8	16(270)	9.1	2.23	971343.0/ 971374.1	0.52	2.75	2.3	1.20			
07-Mar-06	K09->F29	17(152)	8.6	17(100)	8.6	1.81	972122.6/ 972147.7	0.42	2.23	2.1	1.06			
08-Mar-06	C12->H17 ->N06	17(136)	8.3	16(240)	7.4	3.65	972247.4/ 972326.9	1.33	4.98	5.0	1.00			
13-Mar-06	J20->O13	17(136)	8.0	16(250)	7.3	3.20	972781.5/ 972806.8	0.42	3.62	3.0	1.21			
14-Mar-06	E06->H25 ->F19->P22	17(124)	7.7	16(194)	7.5	4.91	972903.1/ 972976.8	1.23	6.14	5.4	1.14			
	Data not shown from 15 Mar 2006 to 26 Sep 2007													
27-Sep-07	L28->M07 ->J20->E18	16(320)	9.2	16(158)	9.2	5.98	1022163.8/ 1022250.3	1.44	7.42	6.7	1.11			
15-Oct-07	R14->C18	16(260)	9.4	16(228)	9.4	1.22	1023283.3/ 1023310.6	0.46	1.68	1.3	1.29			
06-Nov-07	M03->D17 ->H13	17(180)	7.1	16(275)	9.4	4.23	1024863.4/ 1024901.2	0.63	4.86	4.9	0.99			
09-Nov-07	B15->L04 ->H17	16(280)	9.4	16(185)	9.4	3.95	1025215.7/ 1025255.1	0.66	4.61	4.7	0.98			
	Mean													
								Sta	indard De	eviation	<u>+</u> 0.099			

Note 1: "Position" refers to the bottom position of control rod, and AR3 stands for Adjustor Rod No. 3.

Note 2: NRU operates normally between Control Rod No. 16 and No. 17 (between 50 cm and 350 cm for each).

## 6. Conclusions

Several conclusions can be drawn from the above three validation exercises:

- 1) The agreement between the flux detector measurements and simulated fluxes for a variety of axial flux distributions at three monitoring sites of P18, E22 and L06 was fairly good, within  $\pm 6.5\%$ . However, this validation exercise did not cover those distributions with extreme thermal flux depression in the central region of the core.
- 2) Relative to power measurements, it was found that TRIAD3 over-predicted driver fuel rod power by 1.0 %, and the standard deviation for the measured-to-simulated power ratios was ±6.1%. The Mo-99 production rod power was under-predicted by 14.1 %, with a standard deviation of ±9.3%. The standard deviations for loop fuel strings are smaller than for driver rods (less than ±4.3 %), due to their better power monitoring systems and locations in the core.
- 3) The third validation exercise is really an inter-comparison of reactivity values calculated by the TRIAD3 code. The comparison showed that TRIAD3 underpredicts the reactivity change for driver fuel shuffles by about 9% on average, and the standard deviation for the measured-to-simulated reactivity ratios, attributed to measurement random error, is about  $\pm 10\%$ .
- 4) Overall, the three validation exercises contribute to the successful qualification of the TRIAD3 code for modelling the NRU reactor.

### 7. References

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