Serpent modelling of pressurized heavy water CANDU reactors

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1. Introduction and brief history of the CANDU reactor

The CANDU (Canadian deuterium-uranium) reactor refers to several generations of pressurized heavy water reactors developed by Atomic Energy of Canada Limited (AECL) together with Canadian power companies. The first prototype was the NRX (National Research Experimental) reactor which went operational in 1947. This reactor was a pure research reactor moderated by heavy water but cooled by light water. The NRX reactor was placed at the Canadian Chalk River Laboratories and was loaded with metallic uranium fuel [1].

In the 1950s the NPD (Nuclear power demonstrator) reactor was being built and it came to be the first power reactor in Canada. This reactor was moderated and cooled by heavy water and had a fuel consisting of uranium dioxide. The NPD was the first reactor type to have the classic circular CANDU fuel of 19 rods, arranged in three rings, with 1 rod in the first (central) ring, 6 rods in the second ring, and 12 rods in the third outermost ring [2]. The configuration can be seen in Figure 1 below.

A similar design, but with almost 10 times higher electrical power was the Douglas Point Reactor. Thus, having an electrical power of ca 200 MW, this reactor belongs to the model CANDU 200 (or CANDU2) [3].

Later, AECL developed larger versions of the CANDU reactor, which included new dimensions and number of fuel pins. The most successful of these reactor models is the CANDU 600 (CANDU6) which is extensively in power operation in Canada and many other countries. Based on the original CANDU6 design many of these reactors have been upgraded to deliver more electrical power, up to 850 MW [4], i.e. the Bruce-1 reactor. Typical for these designs is the fuel bundle consisting of 37 rods in a circular arrangement. Hence, these fuel assemblies consist of four rings; 1 rod in the first (central) ring, 6 rods in the second ring, 12 rods in the third ring and 18 rods in the fourth and outermost ring. The configuration can be seen in Figure 2 below.

Efforts were made to develop a new and even larger design, the CANDU 900 (CANDU9) but this was never realised [5]. Currently, the development work on the CANDU design is focused on small modular CANDU reactors (CANDU SMR). The previous effort to develop an advanced CANDU design within the Gen III+ framework, the Advanced CANDU Reactor (ACR) was cancelled in 2009 due to high costs [6]. Modern CANDU reactors are also normally run with slightly enriched fuel and therefore reach higher burnup than would be the case with natural uranium.

2. Benchmarking of Serpent model against SF-COMPO

In this work, Serpent2 [7] calculations have been made to model different CANDU designs and to compare reactor observables. We have chosen to look at one early CANDU reactor

(NPD) and one late (Bruce-1) and built their respective geometries as infinite lattices in Serpent2. Both the NPD and the Bruce-1 have reported operational histories as well as isotopic compositions of irradiated fuel to the NEA database SF-COMPO [8] and these reports have been used as experimental data to compare the calculated results to.

The final part of this work presents Serpent calculations for the Pakistani KANUPP reactor where no isotopic data exits to compare to. The Pakistani KANUPP-1 reactor was a CANDU 200 sold by Canada to Pakistan and has been used in Pakistan's for energy production [4]. Pakistan made two nuclear weapons tests in 1998, and for this reason, the reactor fleet of Pakistan is of interest for studying the possible plutonium production capabilities. It should be noted that it has never been unambiguously proven that material from KANUPP was used for weapons purposes, and the calculations included in this work are intended as an exercises using the model benchmarked against the Canadian power reactors NPD and Bruce-1.

3. NPD – Nuclear Power Demonstrator reactor

The nuclear power demonstration reactor (NPD) was a prototype reactor for the subsequent Canadian CANDU reactors and the first power reactor in Canada. It was situated in Rolphton near Chalk River, Ottawa, Canada, and started producing electricity in June 1962, co-owned by Atomic Energy of Canada Limited, Ontario Hydro and Canadian General Electric. The reactor was foremost a research reactor intended for engineering research and knowledge development and training and was closed in 1987 after having achieved its operational goals. [9].

Features of the NPD were that it was a heavy-water cooled and moderated design featuring online refueling of natural uranium. The fuel rods were contained inside pressure tubes with a total of 132 fuel channels. The maximum electric power was 20 MWe.

The data present in the SF-COMPO database for the NPD reactor were reported in 1971 [10]. In the experiment, several samples from rods from all three rings were extracted and dissolved, and the isotopic contents measured with mass spectrometry. The atomic ratios reported are:

Atomic ratio (mol/mol)	U235/U238
Atomic ratio (mol/mol)	Pu239/Pu
Atomic ratio (mol/mol)	Pu240/Pu
Atomic ratio (mol/mol)	Pu241/Pu
Atomic ratio (mol/mol)	Pu242/Pu
Atomic ratio (mol/mol)	Pu/U

The strategy in this work is to implement physical and operational data from [10] and SF-COMPO in an infinite lattice model built in Serpent 2 and simulate the same operation to be able to compare the modelled results of the six atomic ratios above to the experimental ones.

3.1 Reactor design and modelling parameters as reported for the experimental campaign

The NPD fuel assembly consists of fuel rods in a circular arrangement (see Figure 1). In the Serpent calculation, the fuel rod is modelled as a fuel pin cladded by Zircalloy. 19 rods and grouped together in a pressure tube filled with the coolant (heavy water), and the pressure tube is places in a calandria tube made of aluminium which delimits the fuel assembly. Surrounding the assemblies is the moderator, also heavy water.

Inside the assembly are several fuel bundles stacked on top of each other, but this is of no importance in the calculations, since they are performed as an infinite lattice in two dimensions (xy), i.e., the length of the assembly (number of bundles) is in the z direction.

Fuel bundle	
Fuel pin radius	0.7145 cm
Cladding inner radius	0.7195 cm
Cladding outer radius	0.7625 cm
Number of pins in bundle	19
Number of fuel rings	3
Radius of 1st ring (1 pin)	0
Radius of 2nd ring (6 pins)	1.656 cm
Radius of 3rd ring (12 pins)	3.1995 cm
Angular offset 3rd ring	15 °
Pressure tube inner radius	4.14 cm
Pressure tube outer radius	4.572 cm
Calandria tube inner radius	5.08 cm
Calandria tube outer radius	5.208 cm
Lattice pitch	13.0175 cm

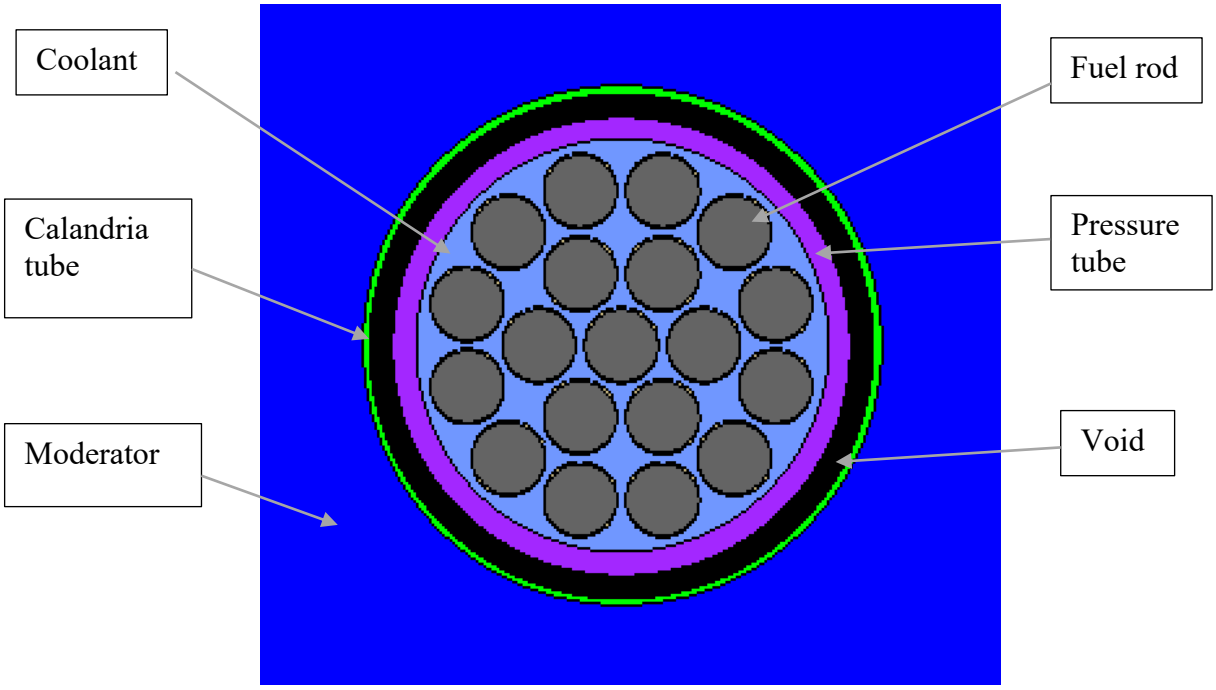

Figure 1. A cross section of the NPD fuel assembly geometry

Materials	**Composition**	**Density (g/cm^3)**
Fuel	Natural uranium dioxide	10.47
Cladding	Zircalloy-4[1]	6.56
Pressure tube	Zr2.5Nb[2]	6.44
Calandria tube	Al	2.7
Coolant	Heavy water	0.863*
Moderator	Heavy water	1.083*

[1]Material definition for Zircalloy-4

Element	**Weight-%**
Sn	1.4
Ni	0.007
Fe	0.15
Cr	0.1
O	0.12
Zr	98.223

[2]Material definition for Zr2.5Nb

Element	**Weight-%**
Nb	2.5
O	0.14
Zr	97.36

* The coolant is kept at high pressure, in the NPD reactor the coolant pressure is 7.2 MPa, for more modern CANDU design the coolant pressure is closer to 10 MPa. The moderator is kept at low pressure and low temperature.

Temperatures		
Fuel	683 K	
Coolant	537.5 K	Avg inlet and outlet
Moderator	311 K	

Other Serpent settings	
Thermal scattering libraries	therm hwtr 0 hwj3.00t hwj3.11t
Cross section data	set acelib "sss_jeff311u.xsdata"
	set declib "/usr/local/SERPENT/endf-b-vi-8_decay.dat"
	set nfylib "/usr/local/SERPENT/endf-b-vi-8_nfpy.dat"
Boundary condition	3 (periodic)

Operating parameters	**SF-COMPO**	**Serpent**
Power density	9.991 W/gUi	9.991 E-3 kW/gU
Power history	620.55 days of power	Daysteps: 100*6 + 20.55
Number of rods analyzed	3	
Burnup rod 1 (est)	5.3 GWd/tU	
Burnup rod 2 (est)	5.6 GWd/tU	
Burnup rod 3 (est)	6.6 GWd/tU	

All geometry and material data in the tables above are taken from [8].

The three rods analysed in SF-COMPO are taken from rings 1, 2 and 3 respectively. Simulations in Serpent were performed both for a full bundle (obtaining average values of all parameters), and for the three rings separately.

4. Bruce-1

Bruce-1 is one of eight CANDU reactors at the Bruce Nuclear Generating Station on Lake Huron in western Ontario, Canada [11].

The Bruce power reactors all belong to the largest running CANDU reactors, with electric power of around 800 Mwe. Bruce-1 started producing power in 1977 and operated until 1997 when the reactor was suspended until 2012 for a major refurbishment campaign. During the years 1998-2012 the steam generator was replaced, upgrades were made to the turbines, and several other changes in order to prolong the reactor's lifetime were employed. The expected lifetime is now until 2043.

The Bruce-1 data in SF-COMPO is from 1995, i.e., before the refurbishments, but still represent a large CANDU reactor. The philosophy behind choosing Bruce-1 besides the NPD reactor is to verify the Serpent model is valid for different sizes of CANDU designs.

The experimental data in SF-COMPO for Bruce-1 are:

Atomic ratio (mol/mol)	U235/U
Atomic ratio (mol/mol)	U236/U
Atomic ratio (mol/mol)	U238/U
Atomic ratio (mol/mol)	Pu239/Pu
Atomic ratio (mol/mol)	Pu240/Pu
Atomic ratio (mol/mol)	Pu241/Pu
Atomic ratio (mol/mol)	Pu242/Pu

Samples were taken from one assembly from three different rods. The Bruce fuel is different from the NPD reactor fuel and has four rings and a total of 37 fuel pins per assembly. The central ring has 1 pin, the second ring has 6 pins, the third ring has 12 pins and the fourth and outermost ring has 18 pins. In [12] it was reported that the three analyses rods were form rings 2, 3, and 4, i.e., the central pin was not analysed.

4.1 Reactor design and modelling parameters as reported for the experimental campaign

The basic design of the fuel is similar to the NPD, but with one extra ring of fuel rods.

Fuel bundle	
Fuel pin radius	0.6075 cm
Cladding inner radius	0.6114 cm
Cladding outer radius	0.6544 cm
Number of pins in bundle	37

Number of fuel rings	4
Radius of 1st ring (1 pin)	0
Radius of 2nd ring (6 pins)	1.4885 cm
Radius of 3rd ring (12 pins)	2.8755 cm
Radius of 4th ring (18 pins)	4.3305
Angular offset 3rd ring	15 °
Pressure tube inner radius	5.169 cm
Pressure tube outer radius	5.603 cm
Calandria tube inner radius	6.448 cm
Calandria tube outer radius	6.5875 cm
Lattice pitch	14.2875 cm

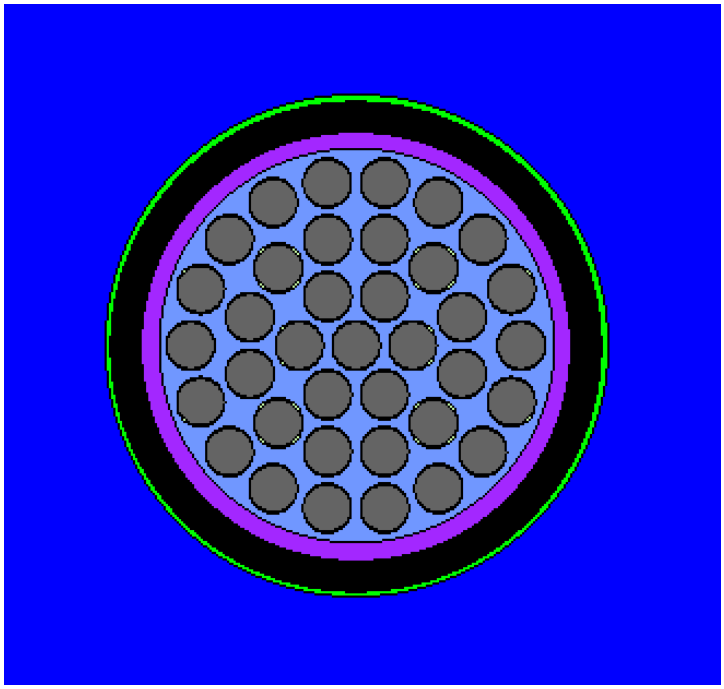

Figure 2. A cross section of the Bruce-1 fuel assembly geometry. See Figure 1 for legend.

Materials	**Composition**	**Density (g/cm^3)**
Fuel	Natural uranium dioxide	10.6
Cladding	Zircaloy-4[1]	6.56
Pressure tube	Zr2.5Nb[2]	6.44
Calandria tube	Zircaloy-4	6.56
Coolant	Heavy water	0.863*
Moderator	Heavy water	1.083*

[1,2] See material definitions above under NPD.
* The coolant is kept at high pressure, in the Bruce-1 reactor the coolant pressure is 9.81 MPa. The moderator is kept at low pressure and low temperature.

Temperatures		
Fuel	1155 K	
Coolant	547.5 K	Avg inlet and outlet
Moderator	346 K	

Other Serpent settings	
Thermal scattering libraries	therm hwtr 0 hwj3.01t hwj3.11t
Cross section data	set acelib "sss_jeff311u.xsdata"
	set declib "/usr/local/SERPENT/endf-b-vi-8_decay.dat"
	set nfylib "/usr/local/SERPENT/endf-b-vi-8_nfpy.dat"
Boundary condition	3 (periodic)

Operating parameters	**SF-COMPO**	**Serpent**
Power density	See power cycle below	See power cycle below
Power history	See power cycle below	See power cycle below
Number of rods analyzed	3	
Burnup rod 1 (est)	7.8 GWd/tU	
Burnup rod 2 (est)	7.8 GWd/tUi	
Burnup rod 3 (est)	7.8 GWd/tUi	

All geometry and material data in the tables above are taken from [8].
Operating history and implementation in Serpent2:

Time (days)	**Power density (kW/g)**
31.63	0.00104
13	0.0301
10	0
43.25	0.03021
55.3	0
49.75	0.0303
9	0
50.33	0.0303
15	0
103	0.0303
3	0
117.25	0.00087

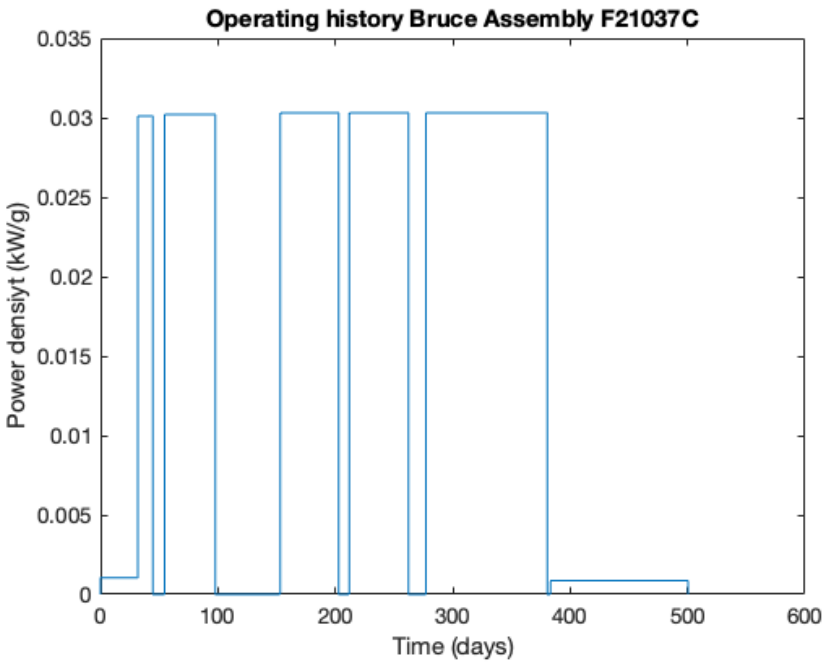

Figure 3. Operating history for the measured samples from Bruce-1.

Modelling of the Pakistani KANUPP reactor

The KANUPP reactor, or Karachi Nuclear Power Plant-1is a 137 MWe CANDU-reactor modelled after the Canadian Douglas Point reactor. KANUPP was acquired by Pakistan in 1971 in a bilateral cooperation with Canada and was in operation between 1972 and 2021.

5.1 Reactor design and modelling parameters for KANUPP

Physical design data on KANUPP can be found in references [2,13-15]

Fuel bundle	
Fuel pin radius	0.71185 cm
Cladding inner radius	0.719 cm
Cladding outer radius	0.757 cm
Number of pins in bundle	19
Number of fuel rings	3
Radius of 1st ring (1 pin)	0
Radius of 2nd ring (6 pins)	1.66 cm
Radius of 3rd ring (12 pins)	3.32 cm
Angular offset 3rd ring	15 °
Pressure tube inner radius	4.1485 cm
Pressure tube outer radius	4.5815 cm
Calandria tube inner radius	5.0625 cm
Calandria tube outer radius	5.2065 cm
Lattice pitch	11.7475 cm

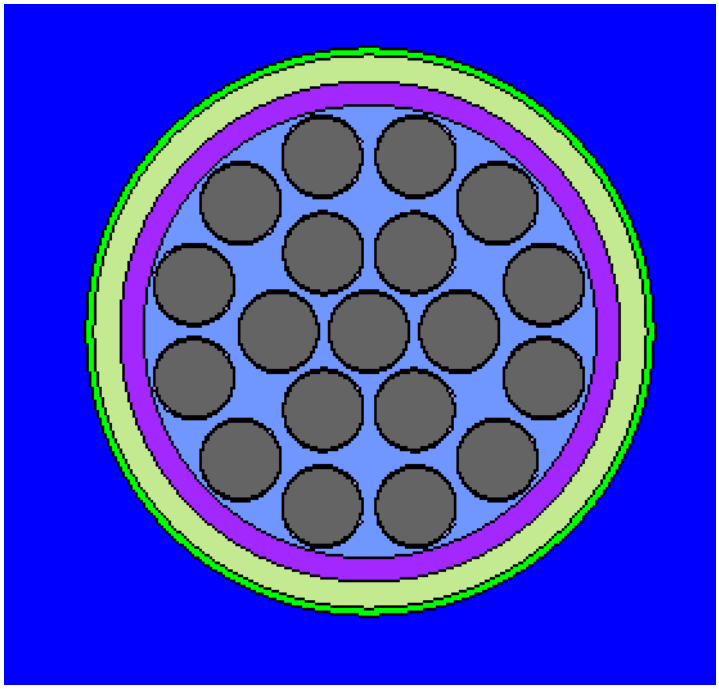

Figure 4. A cross section of the KANUPP fuel assembly geometry. See Figure 1 for legend. Instead of void, the space between the pressure tube and the Calandria tube is filled with CO_2.

Core	
Number of bundles in assembly	11
Number of assemblies	208
Total number of bundles	2288
Uranium per bundle	13.395 kg
UO_2 per bundle	15.221 kg
Uranium in core	30648 kg
UO_2 per bundle	34827 tons

For the KANUPP reactor, we are specifying the number of bundles in the assemblies, as well as the amount of uranium in the core. This information is needed for the calculation of the total amount of plutonium that can be produced.

Materials	**Composition**	**Density (g/cm^3)**
Fuel	Natural uranium dioxide	10.47
Cladding	Zircalloy-4[1]	6.56
Pressure tube	Zr2.5Nb[2]	6.44
Calandria tube	Zircalloy-2[3]	6.56
Coolant	Heavy water	0.863*
Moderator	Heavy water	1.083*

[1,2] See material definitions above under NPD.

[3]Material definition for Zircalloy-2

Element	Weight-%
Sn	1.4
Ni	0.006
Fe	0.14
Cr	0.1
O	0.12
Zr	98.18

Temperatures		
Fuel	683 K*	
Coolant	537.5 K*	Avg inlet and outlet
Moderator	311 K*	

* Pressures and temperatures of the coolant and moderator are taken from the NPD example.

Other Serpent settings	
Thermal scattering libraries	therm hwtr 0 hwj3.00t hwj3.11t
Cross section data	set acelib "sss_jeff311u.xsdata"
	set declib "/usr/local/SERPENT/endf-b-vi-8_decay.dat"
	set nfylib "/usr/local/SERPENT/endf-b-vi-8_nfpy.dat"
Boundary condition	3 (periodic)

Operating parameters	
Power density	11 E-3 kW/gU
Power history	Bustep 5*0.2 + 5*0.1

6. Results

6.1 Benchmarking the NPD reactor when modelling the bundle as one unit

As discussed above, the fuel design is a circular configuration with 1 central pin making up the innermost ring, 6 pins in ring two, and 12 pins in ring three. When calculating the average of the isotopic ratios over the whole fuel bundle, the weighted average has been used, taking into account that fraction of the total fuel in each ring

Table 1: The experimental isotopic results from SF-COMPO and Serpent

Isotopic ratios	Rod 1 1st (central) ring	Rod 2 2nd ring	Rod 3 3rd ring	Weighted average all rods	Serpent
U235/U238	0.003485	0.003252	0.002596	0.00285	0.00257
Pu239/Pu	0.7743	0.7595	0.7189	0.73464	0.726
Pu240/Pu	0.1921	0.2031	0.23	0.21951	0.233

Pu241/Pu	0.02899	0.03174	0.04163	0.03784	0.0413
Pu242/Pu	0.00458	0.00558	0.0095	0.00800	0.0862
Pu/U	0.00271	0.00286	0.00331	0.00314	0.00332

These data are plotted in the figures below

In all reported experimental isotopic ratios, the reported uncertainty was 1% or less. In the plots below, errors of 1% have been indicated in all data points.

The burnup is as described in the table above different for the three rods. The total (average) burnup reached in Serpent with the power history above was 6.2 GWd/tU.

A common way to visualise the deviations between experimental and calculated values is to plot a histogram with the calculated C/E-1:

$$\frac{C}{E} - 1 = \frac{calculated\ (simulated) value}{experimental\ valu} - 1$$

Plots showing the C/E-1 are shown for each simulated reactor.

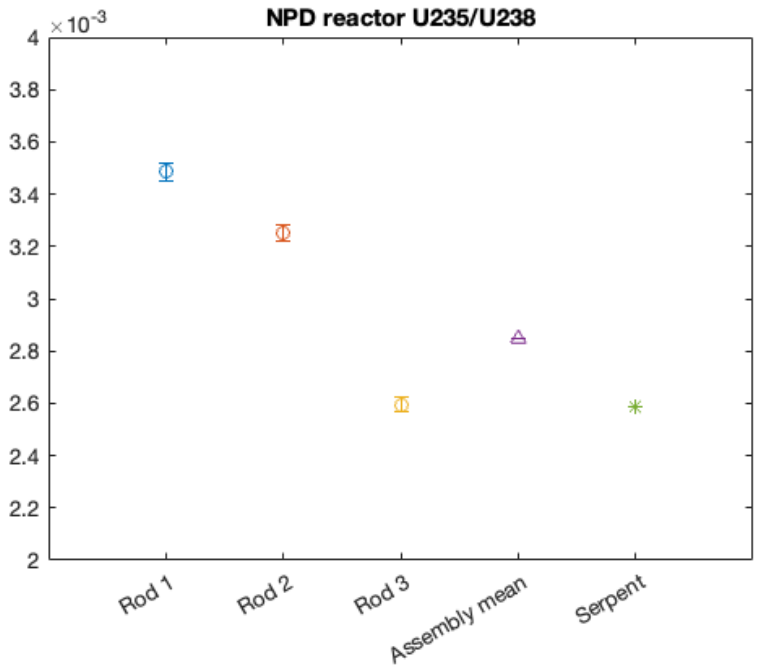

Figure 5. Comparison between the experimentally determined fraction of U235 to U238 in the three rods, the assembly (weighted mean of the three rods) and the Serpent calculation.

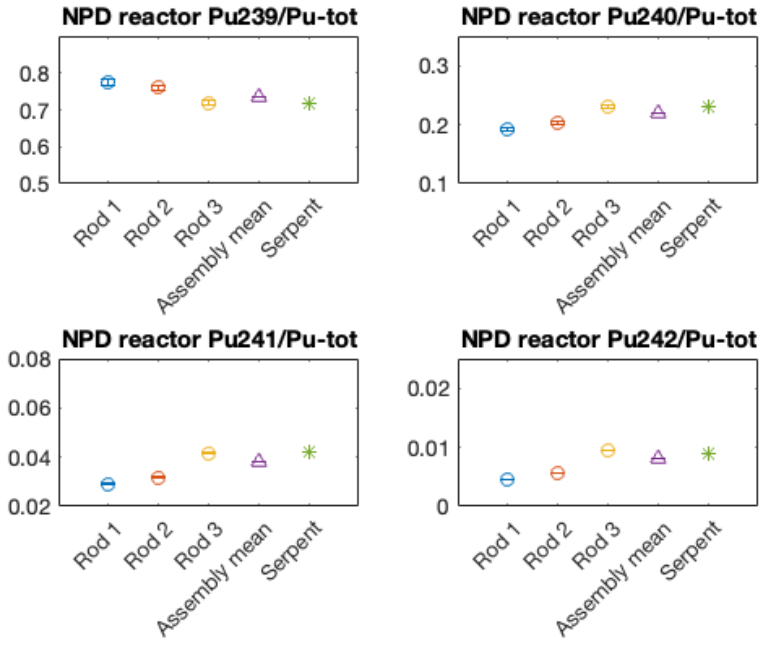

Figure 6. Comparison between the fractions of plutonium isotopes to the total amount of plutonium in the three rods, the assembly (weighted mean of the three rods) and the Serpent calculation

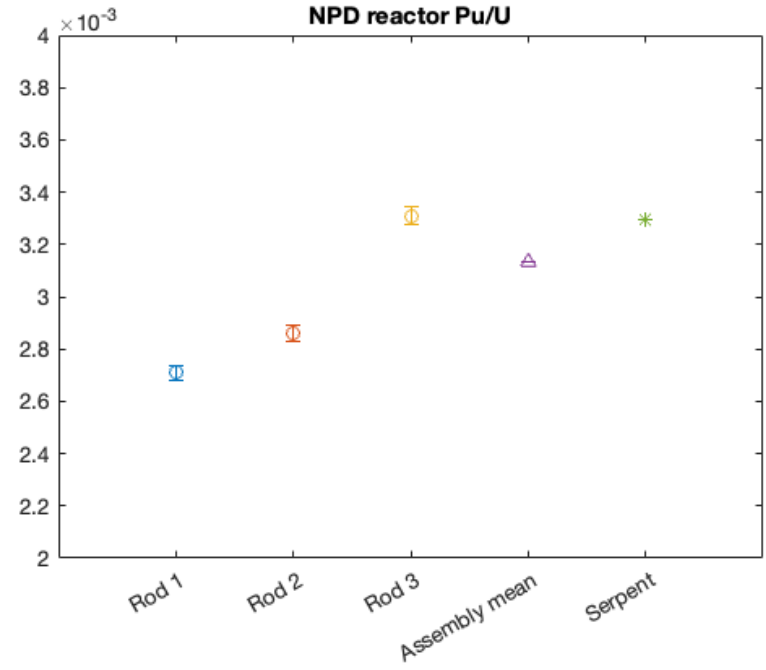

Figure 7. Comparison between the fraction of plutonium to that of uranium in the three rods, the assembly (weighted mean of the three rods) and the Serpent calculation.

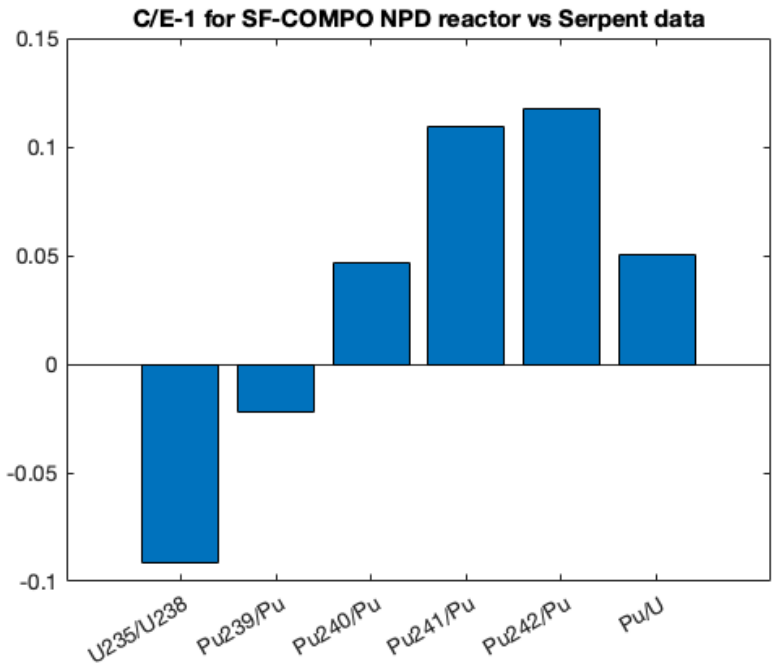

Figure 8. Comparison between calculated (simulated) and experimental results.

6.2 Benchmarking the NPD reactor when modelling the assembly as three separate rings

The operating history of the NPD reactor was also modelled with separated depletion calculations for three different fuel zones corresponding to the three rings in the pin configuration of the assembly. The first zone corresponds to the central pin (the first ring) the second zone corresponds to the second ring and the third zone corresponds to the third ring. With separated depletion calculations, different burnup was obtained for the three rings:

Table 2. Burnups from SF-COMPO and Serpent

	Burnup from SF-COMPO (est)	**Burnup from Serpent**
Rod 1	5.3 GWd/tU	5.0 GWd/tU
Rod 2	5.6 GWd/tU	5.4 GWd/tU
Rod 3	6.6 GWd/tU	6.7 GWd/tU

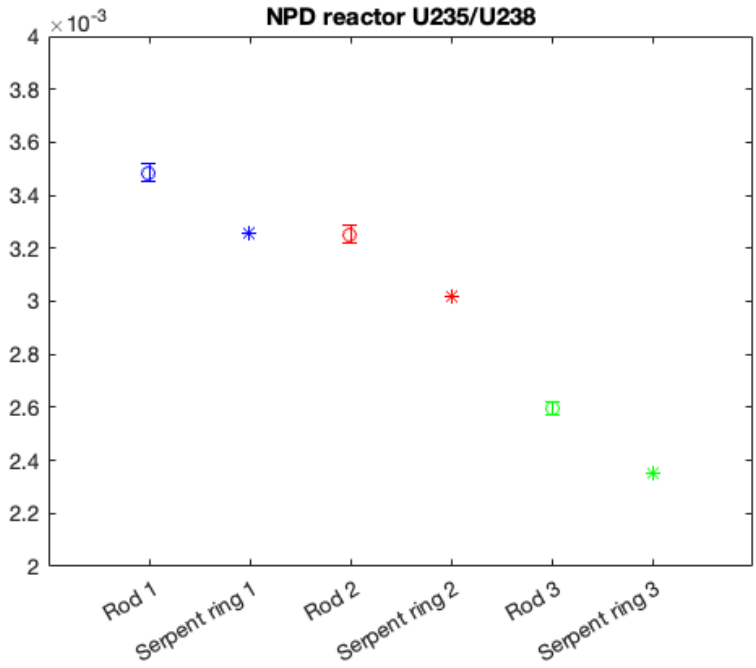

Figure 9. Comparison between the fraction of U235 to U238 in the three rods, and the corresponding ring in the Serpent calculation.

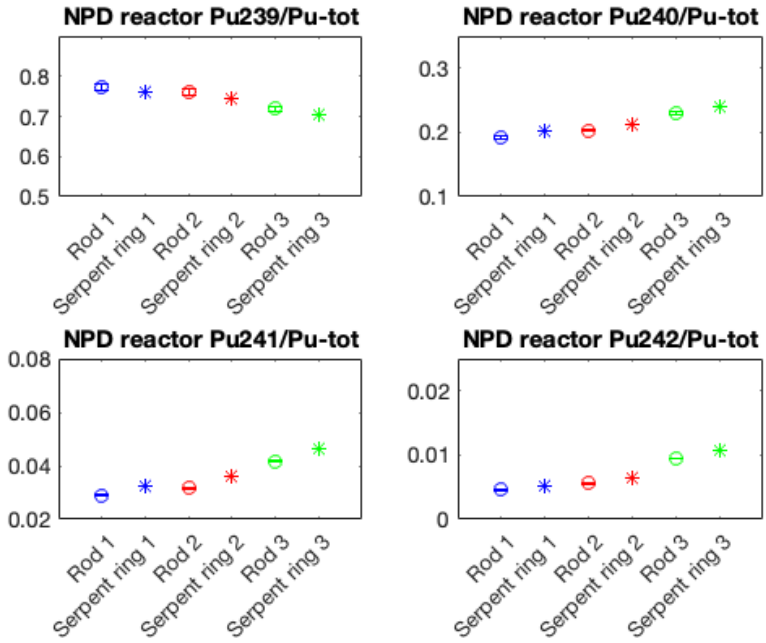

Figure 10. Comparison between the fractions of plutonium isotopes to the total amount of plutonium in the three rods and the corresponding Serpent calculation,

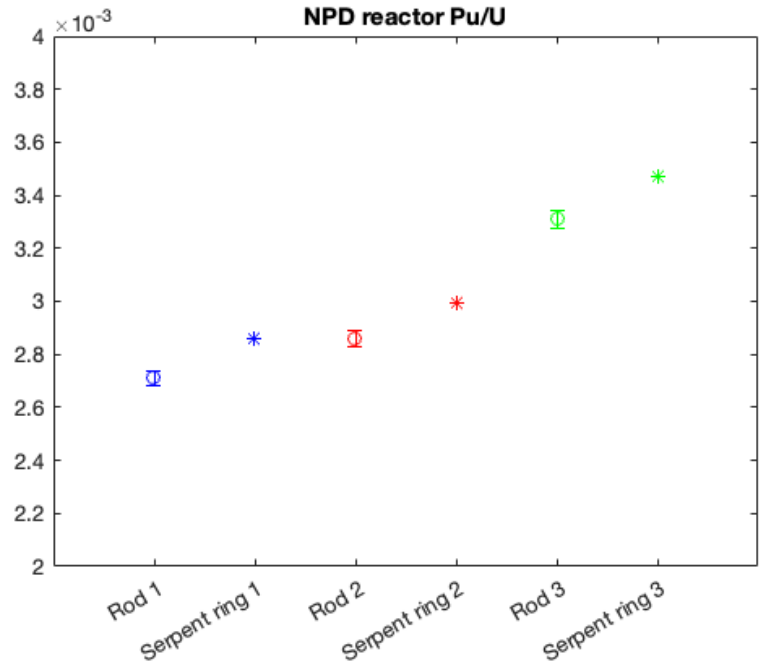

Figure 11. Comparison between the fraction of plutonium to that of uranium in the three rods and the corresponding Serpent calculation.

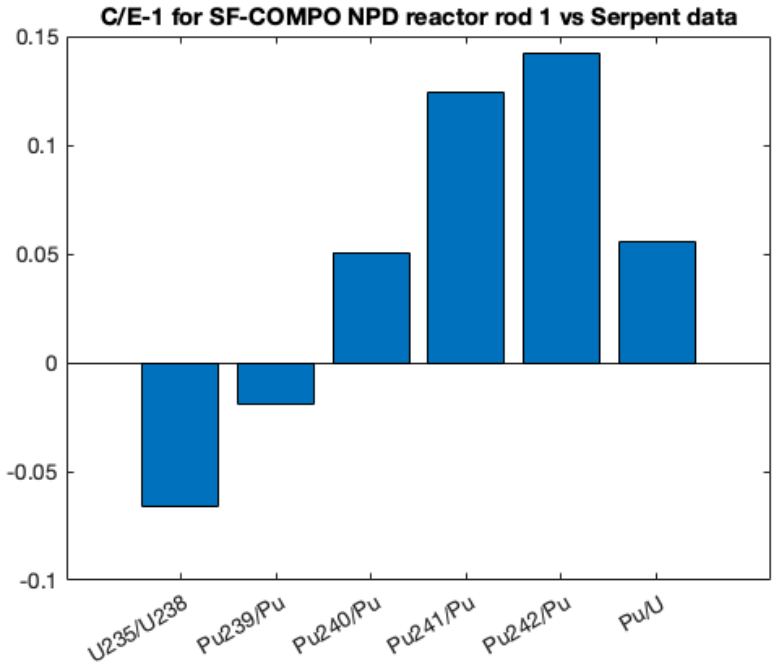

Figure 12. Comparison between calculated (simulated) and experimental results for rod 1.

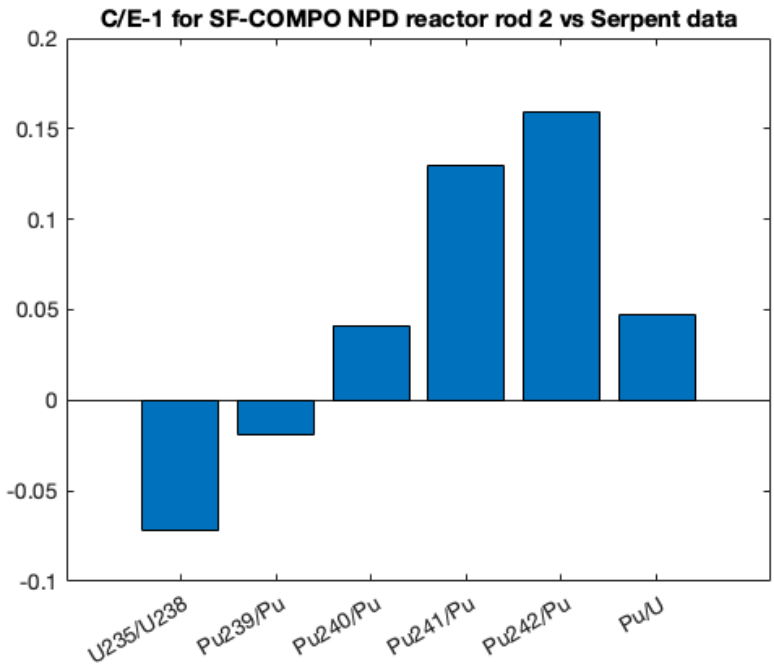

Figure 13. Comparison between calculated (simulated) and experimental results for rod 2.

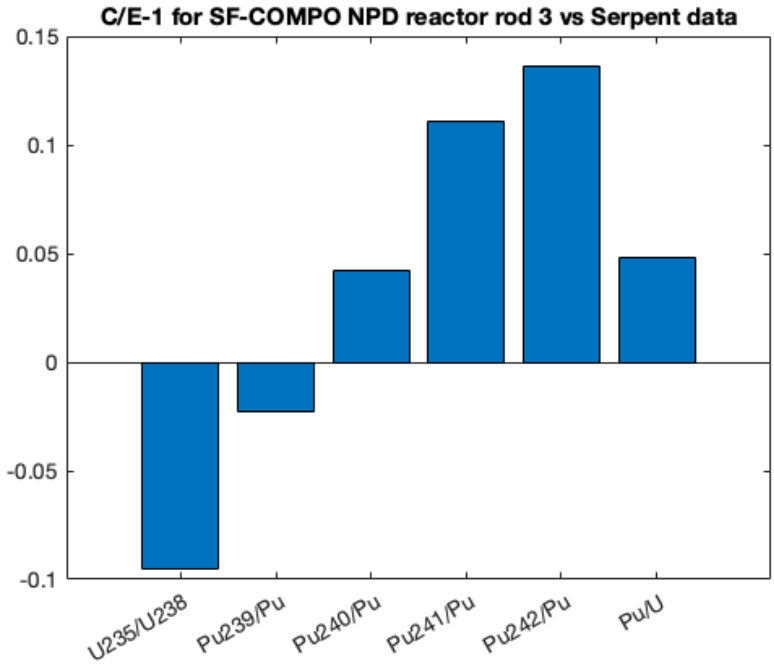

Figure 14. Comparison between calculated (simulated) and experimental results for rod 3.

6.3 Benchmarking the Bruce-1 reactor when modelling the bundle as one unit

In [12] it was reported that the three rods analysed in SF-COMPO rods were from rings 2, 3, and 4, i.e., the central pin was not analysed. Simulations in Serpent were performed for both full bundle (obtaining average values of all parameters), and for the four rings separately. When calculating the weighted average for the SF-COMPO data, it was assumed that the

central ring (the one rod which was not explicitly analysed) had the same composition as the second ring.

Table 3. The experimental isotopic results from SF-COMPO and Serpent (errors in % in parenthesis)

Isotopic ratios	**Rod 1 2nd ring**	**Rod 2 3rd ring**	**Rod 3 4th ring**	**Weighted average all rods**	**Serpent**
U235/U	0.00272 (2.2)	0.00237 (3.4)	0.00174 (5.2)	0.00213 (2.8)	0.00203
U236/U	0.00073 (9.6)	0.00075 (14.7)	0.00087 (5.7)	0.00080 (5.8)	0.00078
U238/U	0.99655 (0)	0.99689 (0.015)	0.99739 (0.1)	0.9971 (0.1)	0.9972
Pu239/Pu	0.7011 (0.3)	0.676 (1)	0.6297 (0.6)	0.6582 (0.4)	0.6595
Pu240/Pu	0.2493 (0.4)	0.2658 (1.9)	0.2903 (1.9)	0.2746 (1.1)	0.2652
Pu241/Pu	0.0393 (4.6)	0.0446 (2.5)	0.057 (4.9)	0.0496 (2,7)	0.0577
Pu242/Pu	0.0103 (6.8)	0.0137 (8.8)	0.023 (7.4)	0.0176 (4.8)	0.0164

The burnup reached in the calculations with the applied operating history was 7.98 MWd/tU.

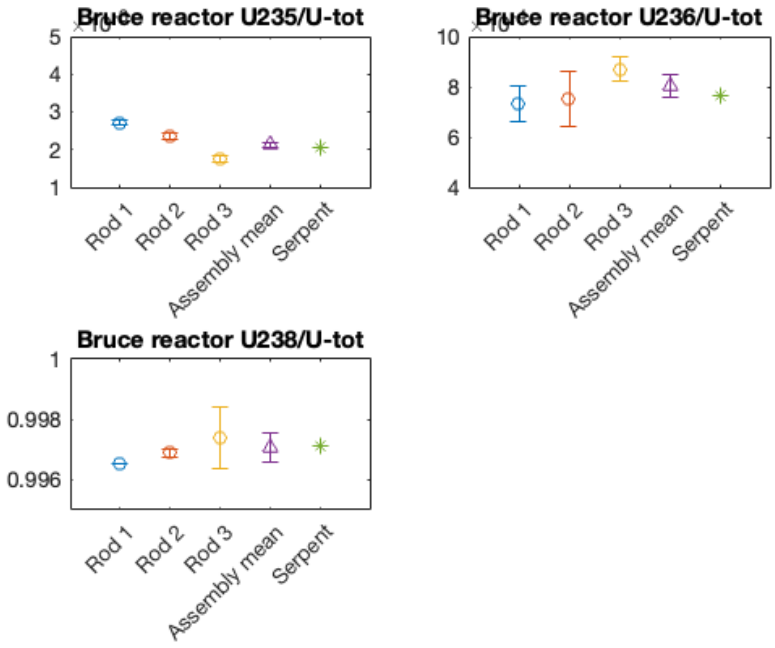

Figure 15. Comparison between fraction of uranium isotopes in the three rods, the assembly (weighted mean of the three rods) and the Serpent calculation.

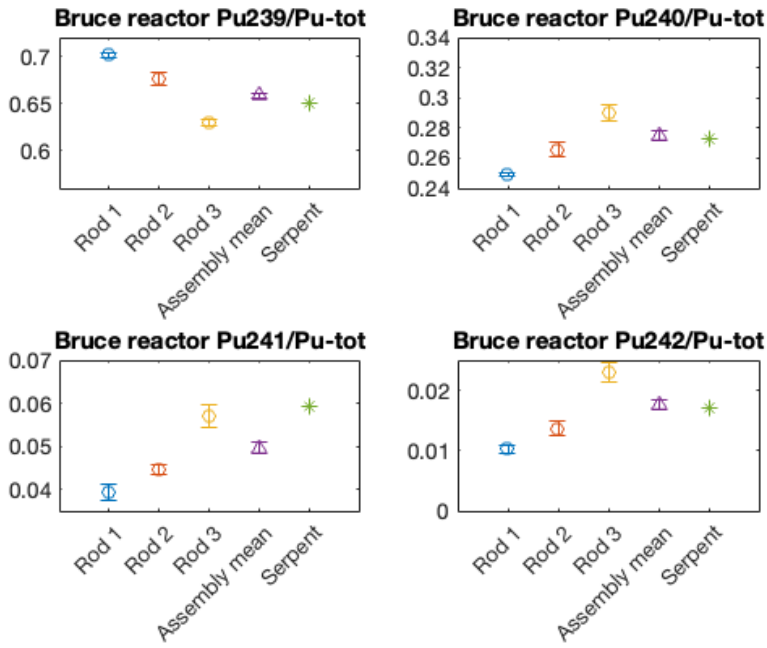

Figure 16. Comparison between fraction of plutonium isotopes in the three rods, the assembly (weighted mean of the three rods) and the Serpent calculation.

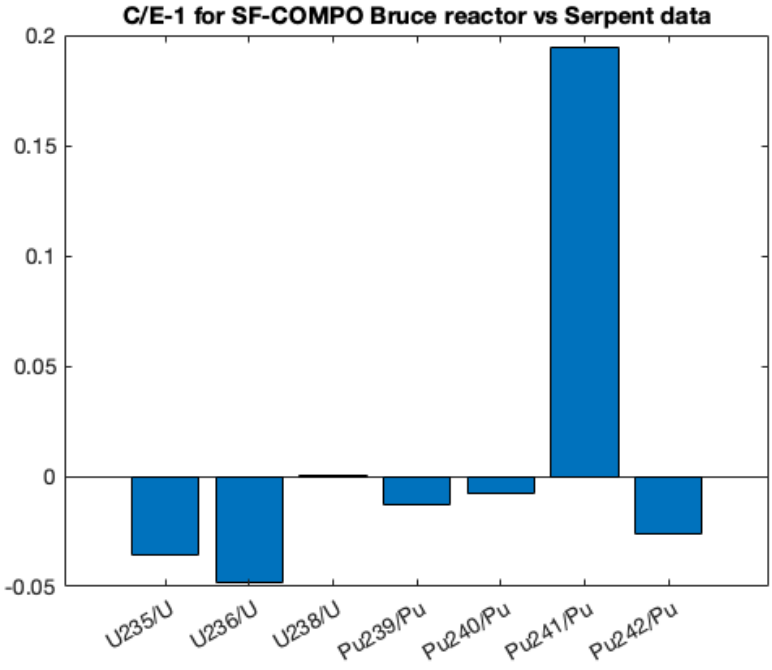

Figure 17. Comparison between calculated (simulated) and experimental results (Bruce)

6.4 Results for the NPD reactor when modelling the assembly as four separate rings

The Bruce fuel consists of four concentric rings and in this section, they have been treated individually, i.e., independent depletion calculations were performed for the four rings. The

resulting burnup were obtained: (note that SF-COMPO does not have information on individual burnup for the three rods).

Table 4. Burnups from SF-COMPO and Serpent

	Burnup from SF-COMPO (est)	**Burnup from Serpent**
Central pin	Not analysed	6.4 GWd/tU
Rod 1	7.8 GWd/tU	6.7 GWd/tU
Rod 2	7.8 GWd/tU	7.4 GWd/tU
Rod 3	7.8 GWd/tU	8.9 GWd/tU
Total average BU	7.8 GWd/tU	8.0 GWd/tU

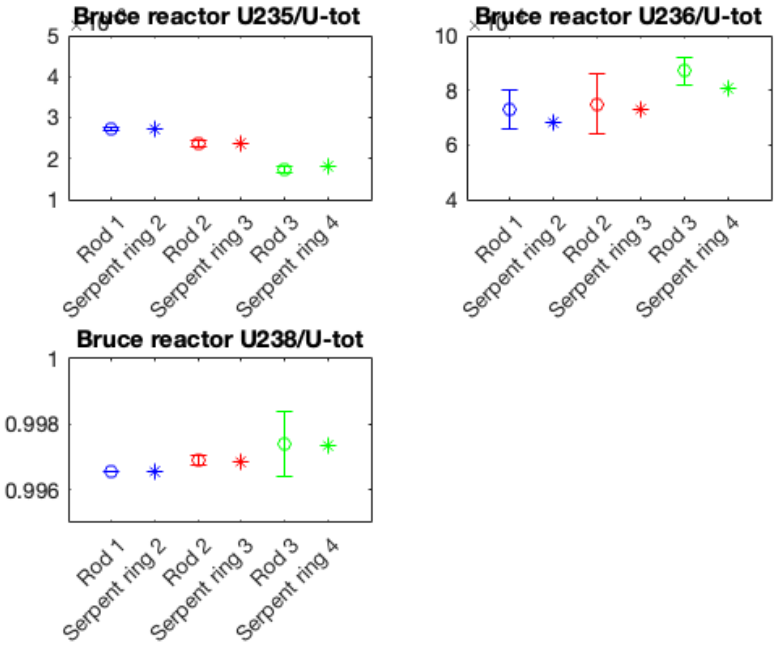

Figure 18. Comparison between the fractions of uranium isotopes in the three rods, and the corresponding rings in the Serpent calculation.

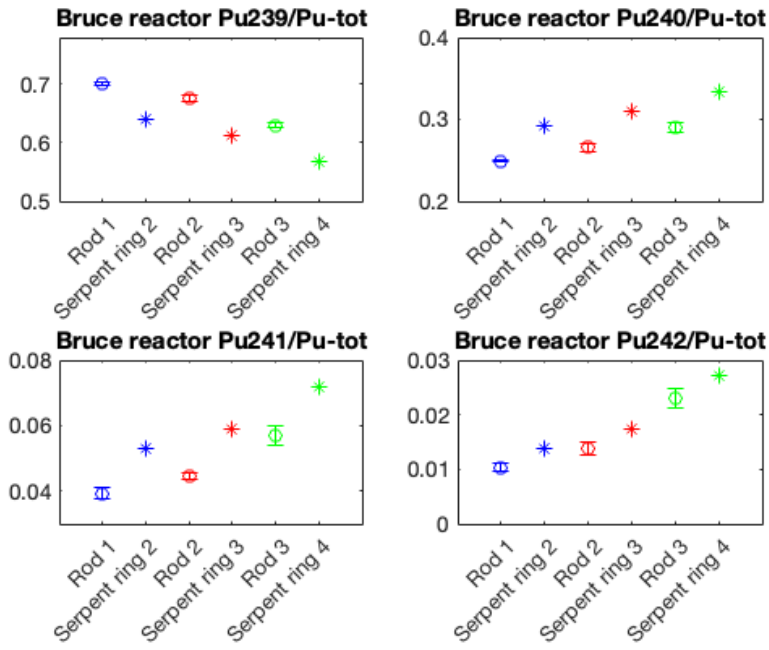

Figure 19. Comparison between the fractions of plutonium isotopes in the three rods, and the corresponding rings in the Serpent calculation.

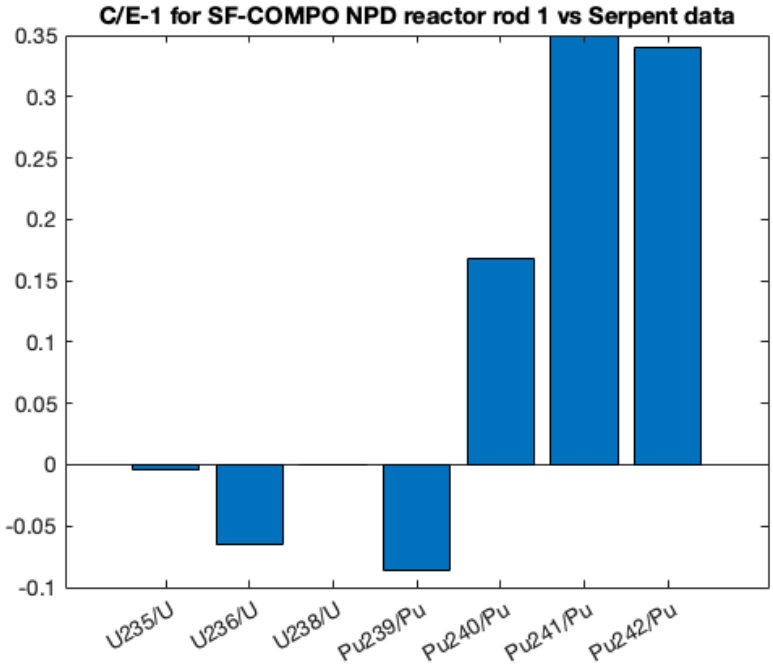

Figure 20. Comparison between calculated (simulated) and experimental results for rod 1.

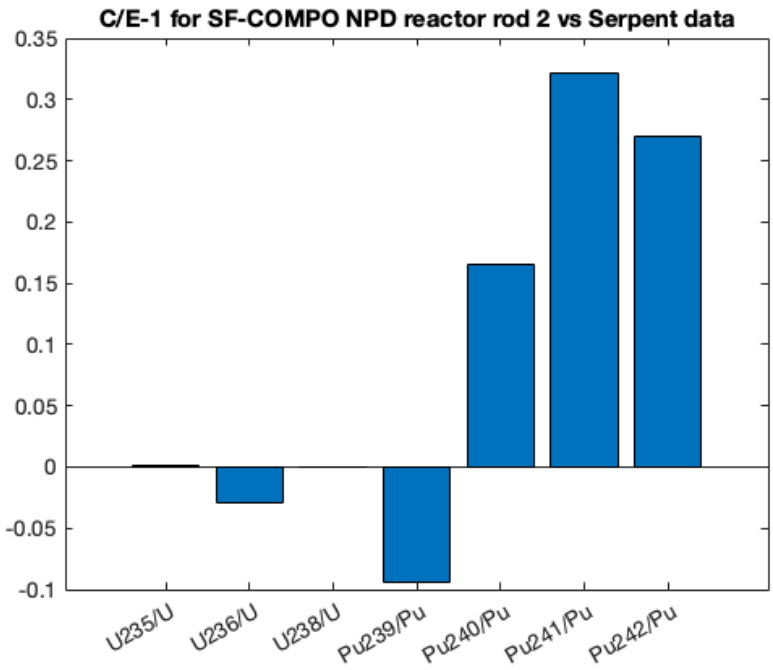

Figure 21. Comparison between calculated (simulated) and experimental results for rod 2.

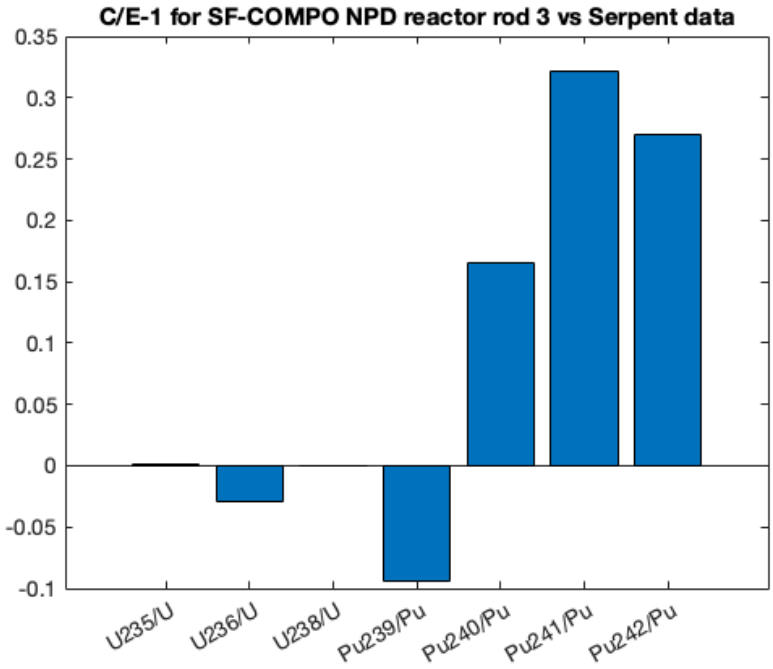

Figure 21. Comparison between calculated (simulated) and experimental results for rod 3.

6.5 Simulation of the KANUPP reactor

When simulating the KANUPP reactor, one interesting observable is to find at which burnup plutonium of weapons grade is obtained, and how much such plutonium can be produced.

Different definitions is used for determining what is meant by weapons-grade plutionium, but here we have used the limit of 93.8 weight-% Pu239. This definition is used i.e., by [16].

In our calculations, the weight-fraction of Pu239 reaches 93.8 % for burnup 1130 MWd/TU. At this burnup the plutonium vector is:

Isotope	Wt%
Pu238	0.0066
Pu239	93.8
Pu240	5.74
Pu241	0.44
Pu242	0.015

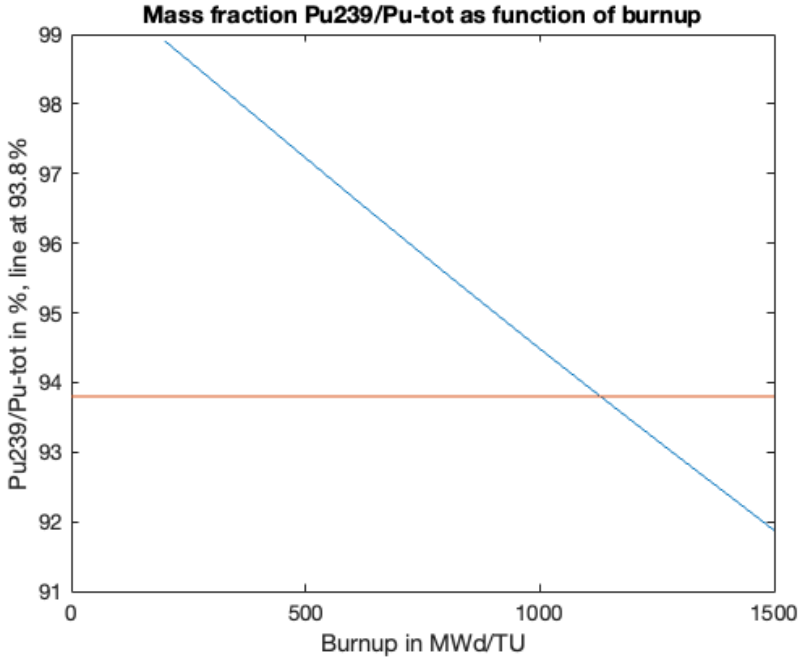

Figure 23. The evolution of the mass fraction of Pu239 as a function of burnup. The red line corresponds to 93.8%

The fraction of plutonium to that of uranium at the reached burnup is 0.0897%.
The total amount of uranium in the core at the BOL is 30648 kg giving the amount of Pu at the burnup calculated above as 27.5 kg or 0.897 kg Pu/TU. Hence, with this operations, the production rate of plutonium (total Pu) is 0.79 g/MWd

7. Conclusion and discussion

7.1 Benchmarking of the Nuclear Power Demonstration reactor

The Nuclear Power Demonstration (NPD) reactor was simulated twice, both with the respect to the fuel as averaged depletion over the assembly and with respect to different depletion in different fuel rings (rods).

To be able to compare the assembly as a whole to the experimental data, a weighted averaged of the isotopic compositions was calculated taking into account the different number of fuel rods in each ring. The Figures 5-7 show plots of the NPD experimental values for the three analysed rods, their weighted average, and the Serpent calculations. From the figures it is obvious that the differences between the rods (from the same assembly) are large, because of differences in neutron fluence and moderation, and with the very small reported experimental errors (< 1%) it is not meaningful to compare the rods to each other. It is also clear the weighted average is dominated by rod 3, coming from the third ring where most of the rods (12 out of 19) are situated. The Serpent values, representing the isotopic ratios for the assembly as a whole, should be compared to the calculated weighted averages in these figures.

C/E-1 is shown for the first NPD calculation in Figure 8. The weighted averages have been used as experimental values, and the Serpent data as calculated. Figure 5 shows fairly good agreement for all isotopic ratios. The Pu239/Pu, Pu240/Pu and Pu/U ratios show a deviation below or around 5 %, and the U235/U238, Pu241/Pu and Pu242/Pu have deviations of around 10 %. The worst case is the heaviest Pu isotope (Pu242) which we can note is the one requiring most calculation and reaction steps in Serpent. It is also created in very small amounts, see Table 1, making the absolute deviation small.

Continuing to the simulations of the individual rings in the fuel, the results for the isotopic compositions are plotted in Figures 9-11. Here, the symbols are to be compared colour-wise, i.e., the blue symbols are the experimental values for rod 1 and the simulated values for ring one, representing the same location in the fuel. In all Figures 6-8 there is a clear trend, that the data points (experimental and simulated) go “the same way”, i.e. in Figure 6 it is noted that the fraction of U235 to that of U238 gets smaller as rods get further from the assembly centre. This also fits with the finding that the burn-up is higher for fuel at larger radii, due to the better moderation.

Figures 12-14 are C/E-1 histograms for the individual rods. Comparing to the assembly mean (Figure 5) the deviations are similar or smaller on a rod-scale for U235/U238, Pu239/Pu, Pu240/Pu and Pu/U and slightly worse for the heavy Pu isotopes Pu241/Pu and Pu242/Pu. In all three rods, the deviations for U235/U238 are negative, which is to be expected since all rings have slightly higher burnup in the simulation than the corresponding experimentally estimated burnups (see Table 2)

7.2 Benchmarking of the Bruce-1 reactor

Also, for the Bruce-1 reactor the simulation was done twice, once with the assembly as a single unit going through the same depletion, and once with separate depletion calculations for each ring in the assembly. Three rods were analysed in the experiment reported in SF-COMPO, and these were taken from rings two- four, i.e., the central rod was not analysed. Consequently, rod 1 corresponds to ring 2, etc.

For the first simulation, with the assembly taken as a whole, the results and comparisons are plotted in Figures 15-17 and the Serpent values should be compared to the weighted averages of the rods, see Table 3. In this calculation, it was assumed that the central pin had the same isotopic composition as the second ring. Note that slightly different isotopic ratios were analysed for Bruce-1 compared to the NPD reactor, and data for the simulations have been chosen to represent what was analysed in the experimental campaign. In Figures 15-16, the

agreements between the experimental assembly mean and the simulated value is good for all isotopes except Pu241. This is also reflected in the C/E-1 histogram in Figure 17, where we can note the deviations are below 5% for all isotopes except Pu241.

The estimated burnup reported to SF-COMPO after the actual operating cycle was 7.8 GWd/tU. In the Serpent calculation a total burnup of 8.0 was reached, explaining the negative deviations for e.g U235/U. Note that in these calculations, the power and operating history were input data and the burnup reached with these parameters was obtained as output.

In the second simulation for Bruce-1, the assembly was divided into its for rings, and they were treated separately with respect to depletion. The comparison between rods and rings can be seen in Figures 18-19, where the symbols of the same colour are to be compared pair-wise. In both the uranium case (Fig. 18) and the plutonium case (Fig. 19) the same trends can be seen when comparing the innermost material (rod 1, ring 2) to the outermost (rod3, ring4). It is expected to see higher burnup at higher assembly radius, but unfortunately, the experimental data set does not report individual burnups for the rods, only an average value, see Table 4.

In the Figures 20-22, the C/E-1 histograms are plotted for each rod/ring. The agreement is worse than in Figure 17 (the whole assembly mean) for all isotopes except U235/U and U238/U.

7.3 The KANUPP simulation

Following the benchmarking of two CANDU designs, The NPD and the Bruce-1, the model for the KANUPP reactor rests on solid ground. The KANUPP reactor is more similar to the NPD reactor and temperature data have been imported from the NPD case to the KANUPP case. Several observables are obtained and can be discussed, but here we have chosen to concentrate on plutonium productions and the possible production rate of weapon-grade plutonium. It should be noted that the KANUPP reactors has never been unambiguously proven to have been producing weapons material, and that power reactors usually have a much (ca five-ten times) higher burnup than the “optimal” burnup for creating weapons-grade plutonium.

Nevertheless, the calculated example shows that substation amounts of plutonium could have been created in the KANUPP reactor, and such operation cannot be excluded.

References

[1] IAEA Research Reactor Database https://nucleus.iaea.org/rrdb/#/home

[2] R.D. Page, *Canadian power reactor fuel, AECL-5609,* 1976 https://canteach.candu.org/Content%20Library/19760101.pdf

[3] *CANDU Nuclear Powe System, AECL, TDS1-105,* 1981 https://inis.iaea.org/collection/NCLCollectionStore/_Public/14/720/14720546.pdf

[4] PRIS – IAEA Power Reactor Information System, https://pris.iaea.org/PRIS/home.aspx

[5] CANDU reactor, https://en.wikipedia.org/wiki/CANDU_reactor

[6] Advanced CANDU reactor, https://en.wikipedia.org/wiki/Advanced_CANDU_reactor

[7] Leppänen, J., et al. (2015) "*The Serpent Monte Carlo code: Status, development and applications in 2013*." Ann. Nucl. Energy, 82 (2015) 142-150, https://doi.org/10.1016/j.anucene.2014.08.024

[8] NEA Database SF-COMPO, https://www.oecd-nea.org/jcms/pl_21515/sfcompo-2-0-spent-fuel-isotopic-composition

[9] https://cns-snc.ca/media/history/npd/historical_backgrounder.html

[10] M.F. Duret, et al., *Plutonium production in NPD: a comparison between experiment and calculation, AECL-3995, 1971, https://www.osti.gov/servlets/purl/4734885*

[11] Bruce Nuclear Generating Station, https://en.wikipedia.org/wiki/Bruce_Nuclear_Generating_Station

[12] I.C. Gauld et al., *Verification and Valiadtion of the ORIGIN-S code and Nuclear Data Libraries, RC-1429*, AECL, 1995, (https://corpora.tika.apache.org/base/docs/govdocs1/856/856807.pdf)

[13] K.M. Wasywich, *Characteristics of Used CANDU Fuel Relevant to the Canadian Nuclear Fuel Waste Management Program, AECL-10463, 1993, https://inis.iaea.org/collection/NCLCollectionStore/_Public/27/002/27002285.pdf?r=1*

[14] IAEA-TECDOC-CD-1751 *Pressurized heavy water reactor fuel: Integrity, Performance, and advanced concepts,* Proceedings of the technical meetings held in Bucharest, 24–27 SSeptember 2012, and in Mumbai, 8–11 April 2013, https://www-pub.iaea.org/MTCD/Publications/PDF/TE_1751_CD/PDF/Tecdoc-1751.pdf

[15] M. Sajjad, et al., *KANUPP Reactor Core Model and its Validation*, 2018 International Conference on Power Generation Systems and Renewable Energy Technologies (PGSRET), Islamabad, Pakistan, 2018, https://doi.org/10.1109/PGSRET.2018.8685948

[16] A. Glaser*, Signatures of Weapon-grade Plutonium from Dedicated Production Reactors,* 49th INMM Annual Meeting, July 13-17, 2008, Nashville, TN, http://www.princeton.edu/~aglaser/CP003-Glaser-2008-INMM-Signatures.pdf