Maintaining a Critical Spectra within Monteburns for a Gas-Cooled Reactor Array by Way of Control Rod Manipulation

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Abstract

This burnup study examined the effect of a predicted critical control rod position on the nuclide predictability of several axial and radial locations within a 4X4 graphite moderated gas cooled reactor fuel cluster geometry. To achieve this, a control rod position estimator (CRPE) tool was developed within the framework of the linkage code *Monteburns* between the transport code MCNP and depletion code CINDER90, and four methodologies were proposed within the tool for maintaining criticality. Two of the proposed methods used an inverse multiplication approach – where the amount of fissile material in a set configuration is slowly altered until criticality is attained – in estimating the critical control rod position. Another method carried out several MCNP criticality calculations at different control rod positions, then used a linear fit to estimate the critical rod position. The final method used a second-order polynomial fit of several MCNP criticality calculations at different control rod positions to guess the critical rod position. The results showed that consistency in prediction of power densities as well as uranium and plutonium isotopics was mutual among methods within the CRPE tool that predicted critical position consistently well. While the CRPE tool is currently limited to manipulating a single control rod, future work could be geared toward implementing additional criticality search methodologies along with additional features.

Keywords: Criticality Search, Critical Spectra, *Monteburns*, Gas Cooled Reactors

1. Introduction

Over the course of operating a nuclear reactor, the isotopic concentration will be altered as isotopes undergo various nuclear reactions and transmutations. Transmutation is proportional to the combination of the temporal neutron flux and macroscopic cross section, where the macroscopic cross section is the product of the microscopic cross section and the isotope atom density. Since isotope atom densities are used to compute the flux, and these atom densities are changing temporally as a function of transmutation, the depletion process is nonlinear. To linearize the depletion calculation, fluxes (or transmutation rates) are computed at a time step, assumed constant and used in a Bateman equation system to progress the atom densities to the next time step. The process then repeats, possibly using a predictor corrector methodology to better approximate the average flux behavior.

In an operating reactor, controlling mechanisms (i.e. control rods, poison solution, etc.) are used to compensate for the loss in reactivity and maintain a self-sustaining chain reaction as the fuel is depleted. These control mechanisms affect both the magnitude and spectra of the energy dependent flux. Because the microscopic cross sections are energy dependent, altering the shape of the energy dependent flux will have a significant effect on further transmutation; and therefore affect buildup and depletion of a particular nuclide. Therefore estimating the critical position and burning with a critical spectra are important for accurate prediction of the temporal nuclide behavior.

The objective of this work is to test the effect of maintaining critical spectra for a graphite moderated gas cooled reactor model through use of control rod manipulation. Most studies that have attempted to address this have been limited to light water reactors and research reactors [1-8]. In this study, four different methodologies for attempting to compute criticality throughout burnup are tested. Because criticality may not exactly be met by each method, the effect on isotope prediction, from slight misprediction of criticality, is also evaluated. Tradeoffs in speed versus accuracy for each method are also investigated. This work is motivated by the need to characterize temporal behavior of graphite moderated gas cooled reactor fuel in the vicinity of, and away from, control rods during operation.

2. Background

The different methods examined in this study for maintaining critical spectra include inverse multiplication methods and polynomial fit methods. A number of reactor design codes currently have an inherent capability of maintaining a critical spectra through a fuel depletion analysis including MC21 [1,9], HELIOS [10,11], McCARD [10,12] and CASMO-3 [2,13]. Davis and Lee [2] performed a depletion analysis of a 17x17 LWR 3.5% enriched UO₂ assembly comparing MCNP5 (coupled with ORIGEN2.2) and MCNPX (coupled with CINDER90) to CASMO-3. The MCNP5-ORIGEN2.2 and MCNPX-CINDER90 links did not contain the capability to maintain critical spectra while CASMO-3 was tested with and without maintaining critical spectra by use of a buckling search. When the buckling search in CASMO-3 was turned off, the three codes matched well enough; however, when the CAMSO-3 buckling search was turned on, the MCNP5-ORIGEN2.2 link over predicted Pu-239 by 6.4% and Pu-240 by 10% while the MCNPX-CINDER90 link over predicted Pu-239 by 11% and Pu-240 by 5%. In their concluding remarks, Davis and Lee [2] stressed the need to repeat the study while accounting for buckling search in the MCNP5-ORIGEN2.2 and MCNPX-CINDER90 links. Yun and Cho also [3] carried out a depletion calculation on an 18x18 UO₂ assembly and MOX assembly. The authors compared a depletion calculation with and without maintaining critical spectra, using albedo (constant incoming and outgoing flux ratio) boundary conditions, and demonstrated minimal difference in isotopic prediction (within

~2.0%) for certain uranium and plutonium isotopes. Though minimal percent difference was realized in actinide prediction, these differences did result in reasonable (~15%) difference in pin power reconstruction at beginning and end of cycle. Park et al. [10] also developed a method to apply a buckling based criticality search to McCARD and then examined the effect of critical spectra on group constants and flux profiles during the depletion calculation using both McCARD and HELIOS. The results showed a disparity of as much as 3.0% when using a critical spectrum in McCARD versus not, and a maximum error of 2% when using a critical spectrum in HELIOS versus not. These methods focused on the effect of maintaining criticality in a truncated geometry by way of adjusting the leakage. When controlling mechanisms are used to maintain criticality, the local effect of the flux shape and magnitude change will affect further transmutation. Therefore it is also important to investigate the effect of movable controlling mechanisms maintaining criticality throughout the burn. Maintaining critical spectra in *Monteburns* through use of control mechanism motion has been examined for rotating drum space reactors [14]; however, that study did not examine different approaches for determining critical position.

Methods of predicting critical position usually involve extrapolation of inverse multiplication, or running a series of calculations and fitting the data to a line or polynomial to extrapolate the critical parameter. Li et al [15] used an initial guess for the reactivity (k_{eff}) and one more criticality calculation, using a differential operator perturbation scheme, in order to fit calculated k_{eff} s to a polynomial to predict critical position. Technically, this method involved computing points and fitting them to a polynomial; however, the amount of total simulations was minimized by gaining two simulations for one through use of the differential operator method. The authors also caveated that the accuracy of the prediction was governed by the accuracy of the particular order Taylor series used to represent the actual perturbation (which may not be known a priori); therefore the main disadvantage of the perturbation operator method was that the effect of the reactivity change would need to be approximated in advance to estimate the order of polynomial needed to extrapolate the reactivity effect. Amiri [16] utilized a curve fitting scheme to a polynomial in order to estimate critical design parameters (i.e. enrichment zoning, fuel pitch, coolant diameter, etc.) for a nuclear thermal rocket design. Authors Loaiza and Gehman [17] chronicled a series of historical critical experiments of which approach to critical was completed by the inverse multiplication (or 1/M) methodology. The 1/M methodology involved experimental measurement of the inverse multiplication factor at separate states with addition of fissile material (or decrease in displacement distance, or increase in reflection). The critical position was extrapolated by using a linear fit to the last two measured data points. If criticality was reached, the process was finished; otherwise, the procedure would repeat until criticality was met. The advantage of polynomial fit methods are that it is easy to fit a few points to a line or curve function and invert the function to determine the critical parameter. The disadvantage of the curve fit methods are that the fitted function may not explicitly compute the actual critical position (as the data is a fit). The advantage of the 1/M methodology is that the critical position will eventually be computed accurately; however, several iterations may be required in order to compute the critical position.

3. Method

A carbon dioxide gas cooled, graphite moderated, Magnesium Non-Oxidizing (Magnox), 4X4 unit cell, was modelled in MCNP6 1.1 Beta [18] to test the critical rod position estimator (CRPE) in the burnup linkage code *Monteburns* [19-21]. This model was derived from a typical graphite moderated gas cooled reactor design [22]. MCNP is a stochastic based radiation transport code that uses continuous energy cross sections and combinatorial geometry to simulate the transport of radiation through matter by the random sampling of events [18]. In MCNP, each path etched by a particle's movement through the

problem domain is called a history. A history starts at birth (from either a fission site in an eigenvalue calculation or source definition in a fixed source calculation) and then can either leak, scatter or capture (or fission in a fixed source calculation) [18]. By tracking the trajectory of many individual particles, the average particle behavior within the medium can be determined as long as the contributing transport phase space has been significantly sampled. At minimum (for transport not in a void), MCNP requires surface cards, cell cards, material definitions and a source definition. Tallies are also implemented to extract data about the transport (i.e. detectors, eigenvalues, reaction rates, etc.). ORIGEN and CINDER90 are point depletion solvers capable of solving the time dependent Bateman equations [23-26]. The input for both ORIGEN and CINDER90 is the number density at time $t=t'$ and destruction and creation coefficients, normalized to thermal power level.

Monteburns [19,21] is a linking script (written in FORTRAN and Perl) that connects MCNP to either ORIGEN or CINDER90. *Monteburns* yields burnup results based on various material feed/removal specifications, power(s), and user specified time steps. *Monteburns* performs one or more MCNP and CINDER90/ORIGEN runs for each user specified time step. While multiple runs per time step increase accuracy, this comes at a great computational expense [19,20]. However, with advances in computational power, the calculation is feasible. For execution, *Monteburns* requires a working MCNP input file and a *Monteburns* input file with user specified depletion parameters [20]. For this particular study, CINDER90 was used as the Bateman solver. CINDER90 possess a 63-group cross section set for 3400 nuclides. MCNP supplies energy integrated reaction rates (creation and destruction coefficients) for a subset of the nuclides for which there are cross sections in MCNP. MCNP also supplies a 63-group flux to be matched with CINDER90 inherent cross sections for those isotopes not tracked in MCNP. The linking process works as follows: (1) MCNP calculates destruction and creation coefficients based on initial atom densities and transport conditions; (2) CINDER90 takes those destruction and creation coefficients and progresses the atom densities to the next time step; and (3) the process repeats. CINDER90 does contain the ability to compute atom densities, activities, delay neutron production rate, cumulative spontaneous fission, absorption, decay and (n,f) reactions of every nuclide at a specified time [23-25]; and *Monteburns* does save all the CINDER90 inputs and outputs per time step for each material.

3.1. MCNP Setup

Figure 1 displays a radial slice of a single pin cell in the geometry, and Figure 2 displays a zoomed out radial and axial profile of the pin cell array. Each fuel pin was 1.46 cm in radius and 101.6 cm in height [22]. The fuel was composed of “natural uranium metal” with a density of 18.7 g/cc (uranium atom fractions by isotope are given in Table 1). Each fuel pin had 3.5 cm Magnox endcaps at the top and bottom.

Table 1. Fuel Composition.

Isotope	Weight %
²⁷ Al	0.1000
²³⁴ U	0.0055
²³⁵ U	0.7193
²³⁸ U	99.1752

The fuel was surrounded by a 0.01955 cm thick Helium (0.5768 mg/cc) gas gap. The Helium density was attained using an average temperature and pressure of 654 K and 6.00 bar [22,27]. The fuel was then clad by a Magnox alloy with a thickness of 0.17 cm and density of 1.74 g/cc [28]. MAGNOX fuel pins normally have fins to facilitate turbulent heat transfer. These fins are very difficult to model explicitly in MCNP. As a result, we simplified the model by assuming a cylindrical clad and did not attempt to model the fins. The fuel pin was then surrounded by a CO₂ (7 mg/cc) coolant channel, which was 5.3 cm in radius. The CO₂ density was attained using an average coolant temperature and pressure 515 K and 6.72 bar [22]. The combination of the fuel pin and coolant channel is termed the “fuel channel”. The fuel channels in the 4X4 unit cell were separated on a square pitch of 20.3 cm with graphite at a density of 1.7 g/cc [29]. The Helium backfill, Magnox clad, CO₂ coolant and graphite moderator isotopic concentrations used in the model are given in Table 2 [30].

Table 2. Additional Isotopic Compositions.

Region	Isotope	Weight %	Region	Isotope	Weight %
Magnox Clad	⁹ Be	2.500E-03	Helium gap	³ He	9.9999E+01
	²⁷ Al	8.000E-01		⁴ He	1.3400E-04
	²⁴ Mg	7.835E+01			
	²⁵ Mg	9.918E+00	CO ₂ coolant	¹² C	2.729E+01
	²⁶ Mg	1.092E+01		¹⁶ O	7.271E+01
	⁴⁰ Ca	7.755E-03			
	⁴² Ca	5.176E-05	Moderator	¹² C	1.000E+02
	⁴³ Ca	1.080E-05			
	⁴⁴ Ca	1.669E-04			
	⁴⁶ Ca	3.200E-07			
	⁴⁸ Ca	1.496E-05			
	⁵⁴ Fe	3.507E-04			
	⁵⁶ Fe	5.505E-03			
	⁵⁷ Fe	1.271E-04			
	⁵⁸ Fe	1.692E-05			

Table 3. Control blade Isotopic Composition.

Isotope	Weight %	Isotope	Weight %
¹² C	8.000E-02	²⁸ Si	6.917E-01
⁵⁵ Mn	2.000E+00	²⁹ Si	3.514E-02
³¹ P	4.500E-02	³⁰ Si	2.319E-02
⁵⁴ Fe	3.583E+00	⁵⁰ Cr	8.256E-01
⁵⁶ Fe	5.624E+01	⁵² Cr	1.592E+01
⁵⁷ Fe	1.299E+00	⁵³ Cr	1.805E+00
⁵⁸ Fe	1.729E-01	⁵⁴ Cr	4.494E-01
⁵⁹ Co	2.000E-01	⁵⁸ Ni	8.510E+00
¹⁴ N	9.964E-02	⁶⁰ Ni	3.278E+00
¹⁵ N	3.640E-04	⁶¹ Ni	1.425E-01
³² S	2.850E-02	⁶² Ni	4.206E-01
³³ S	2.250E-04	⁶⁴ Ni	1.157E-01

³⁴ S	1.275E-03	¹⁰ B	7.960E-01
³⁶ S	3.000E-06		

Each fuel channel was 6.516 m long, housing 6 fuel rods, one on top of the other [22]. The control rod, perforating the center of the 4X4 unit cell was 2.225 cm in radius, and made of boron steel with a density of 7.74 g/cc [31]. The maximum active length of the control rod was 5.4 m with insertion from the top [22]. The control blade composition is shown in Table 3 [31]. The unit cell employed had reflected boundaries in x and y directions and graphite reflection in the z direction. The reflected top graphite section in the z direction was 40 in thick, and the reflected bottom graphite section in the Z direction was 35 in thick. A not to scale diagram is shown in Figure 2.

The temperatures of the uranium fuel, Helium gap, Magnox clad, CO₂ coolant channel, graphite moderator and control blade were 702 K, 654 K, 654 K, 518 K, 516 K, and 516 K respectively [22]. In the MCNP model, these temperatures were accounted for by the combination of using TMP cards evaluated to the exact temperature and using ACE (a compact ENDF) formatted cross sections at the nearest available temperature. The TMP cards in MCNP6 were used to adjust the thermal cell temperature necessary for the free-gas thermal treatment of low-energy neutron scatter [18,32]. The ACE formatted cross sections used for each of the regions were taken from an ENDF/B VII.0 temperature dependent library processed in-house at 50 K increments using the NJOY processing code [33]. Therefore, in the MCNP model, the nearest 50 K library was selected to capture tabular interaction physics while the free-gas scattering was set at the actual operating temperatures (using the TMP cards in MCNP). When a neutron thermalizes (<6 eV), the energy of the bond of the species can affect the interaction kinematics. In MCNP, below 6 eV, if available for a particular species, and selected by the user, S(α,β) cross sections for the entire material replace the individual isotope cross sectioned in order to better capture the effect of the bound species on the interaction kinematics. Due to the extensive amount of graphite, this particular reactor was extremely thermal; and therefore we used the graphite S(α,β) kernel evaluated at 500 K (the in-house 50 K cross section simply uses the S(α,β) available in the official MCNP release) [18,32,33]. Each criticality calculation was run with 10,000 histories per cycle, 30 settle cycles and 270 active cycles.

Figure 1. Close up radial view of a pin cell adjacent to control rod.

Figure 2. Radial and axial view of a 4x4 pin cell array. Fully reflected boundaries in radial view. The axial view shows all 6 fuel elements within a fuel channel, as well as the initial critical control rod position (in dark grey inserted a distance of 4.84 m) relative to the length of the fuel channel.

3.2. Monteburns Setup

This study used *Monteburns* version 3.0 [21]. The volume of each pin and corresponding MCNP material to be burned were specified in the *Monteburns* input. The calculations used 17 time steps. Table 4 displays the time step duration in the left column and cumulative burnup in the right column. The initial time steps were shorter (increments of 100 MWD/MTU) due to the need to gradually attain equilibrium concentrations of Xe-135 and Sm-149, while the later time steps were larger (increments of 1500 - 2000 MWD/MTU). The entire 4X4 system was modeled with a total power level of 1.832 MWt, and was kept at 100% power level throughout all burn time steps (this model does not assume downtime for an outage). Downtime will typically affect shorter lived isotopes such as Eu-154 ($t_{1/2} = 8.6$ years), Cs-137 ($t_{1/2} = 30.2$ years) and Pu-241 ($t_{1/2} = 14.4$ years) [34].

The power level for the system was attained by the product of the total fuel volume and average specific pin power. The average specific pin power for this calculation was 1.5 kW/kg [22]. The buildup of isotopic inventory, specifically actinides, was examined in all 16 fuel channels for all 96 unique fuel pins, as the expectation was that the axial buildup of actinides will vary significantly.

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Table 4. Burnup time steps.

MB time step	MB step-size	Burnup (MWD/MTU)
1	1.00	2
2	10.00	17
3	55.67	100
4	66.67	200
5	66.67	300
6	66.67	400
7	66.67	500
8	66.67	600
9	66.67	700
10	66.67	800
11	66.67	900
12	66.67	1000
13	333.33	1500
14	1000.00	3000
15	1000.00	4500
16	1000.00	6000
17	1333.33	8000

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3.3. The CRPE tool

207 Figure 3 is a schematic of how the CRPE tool was implemented in a typical Monteburns criticality search
208 calculation. The CRPE tool is an “approximate” criticality search routine (written in python) which is
209 called prior to the next burn step, if the criticality search flag is present. When called, a duplicate copy
210 of the latest MCNP file – resulting from a CINDER90 calculation in Monteburns (or “mbmc” file) – was
211 made. The original “mbmc” file was left untouched, and all manipulations completed by the CRPE tool
212 were applied only to the duplicate copy. This duplicate copy of the “mbmc” file also contained the most
213 recent isotopic inventory of all materials being burned. Monteburns usually creates several tallies for
214 computing continuous energy integrated collision rates of various transmutation interactions for use as
215 destruction and creation coefficients in CINDER or ORIGEN. These tallies result in computational
216 burden; therefore during the criticality search algorithm, these tallies were expunged from the
217 duplicate “mbmc” file. After the Monteburns tallies were expunged, several criticality calculations were
218 completed in order to estimate the critical position of the control rod. A source file (or srctp file) was
219 pre-generated for the first instance of the criticality calculation. Subsequent criticality calculations used
220 the source file from the previous calculation such that reasonable guesses of the eigenfunction were
221 recycled. We investigated here both the accuracy and computational burden of using four different
222 algorithms for estimating the actual critical position, within the CRPE tool. A schematic of the CRPE tool

within the Monteburns framework is shown in Figure 4. The different methods for estimating critical position of the control rod within the CRPE tool include:

Figure 3. The *Monteburns* setup with the incorporation of the CRPE tool.

1. The Linear Regression Estimation (LRE): Using 3 user defined control rod positions – 25%, 50% and 75% of the control rod active length in this instance – three separate criticality calculations were initiated using the same setup parameters as initially specified on the input deck. At the conclusion of the calculation, three abscissa data points for the control rod positions, along with three corresponding ordinate k_{eff} values, were used in conjunction with a standard scientific python computing package (numpy library) [35], to perform a linear regression fit and determine the critical rod position [35]. The expectation was that the LRE method would produce consistent results, even though the estimations would not be accurate for all time steps. This was hypothesized because the pure linear relation between reactivity and rod position is not accurate for the full range of burnup [17,36].
2. The Polynomial Regression Estimation (PRE): This technique was identical to the LRE, except instead of using a linear regression technique, a second order polynomial fit from the python numpy library [35] was used to determine the critical rod position. While the expectation was that this approach would be more accurate than the LRE method, because higher order polynomials can be prone to wild oscillations, one hypothesis was that this attribute may actually result in inaccurate critical positions [17,35].
3. Classic Approach to Critical Estimation (CATCE): First, two initial user defined control rod positions – 25% and 75% of the control rod active length in this instance – were evaluated for use in predicting the critical position by traditional linear regression. Then the estimated critical position was evaluated. If the estimated critical position was within 1 standard deviation of critical, the algorithm was finished. If not, then the two calculations closest to critical were used to estimate a new critical position. The algorithm repeated using the two calculations closest to critical to estimate a new critical position until one of the following criteria were met: (1) 5 iterations had elapsed; or (2) attaining a result of critical within one standard deviation [17,35].

A linear regression approach with small changes in reactivity for subsequent iterations has historically been the most prudent choice for an approach to critical [17]. The expectation was that this would be the most accurate of all three methods used by the CRPE tool, subject to the number of maximum iterations allowed.

4. Modified Approach to Critical Estimation (MATCE): Like the CATCE method, the same initial user defined control rod positions were evaluated for use in predicting the critical position by traditional linear regression. Then the estimated critical position was evaluated. If the estimated critical position was within 1 standard deviation of critical, the algorithm was finished. If not, then the closest subcritical calculation (to critical) and closest supercritical calculation (to critical) were used to estimate a new critical position. The algorithm repeated this process until either 5 iterations had elapsed or until attaining a result critical within one standard deviation [17,35]. If a subcritical calculation did not exist, then a backup calculation with the rods fully inserted was invoked. If a supercritical calculation did not exist, a backup calculation with the rods fully withdrawn was invoked. This method was developed primarily as an alternative to the CATCE.
5. No Criticality Search (NCS): The NCS method was currently how *Monteburns* was configured to run by default, i.e. the criticality search flag was turned off. In the NCS, the calculation was carried out with the control blade fully withdrawn.
6. Initial Criticality Search (ICS): At its 0th time step, the ICS method used a hardcoded initial critical rod position (derived from CATCE). The control blade was subsequently kept at the same position throughout the rest of the burnup calculation.

After the critical rod position was determined, the original (and untouched) “mbmc” file was updated with the new critical rod position, and the code proceeded to the next burn time step.

○ Rod positions — PRE LRE --- ATCE

Figure 4. Schematic of critical position estimation techniques.

4. Results

The graphite reactor model developed in section 3.1 was used to test the capabilities of the different criticality search methods within the CRPE tool. Figure 5a displays the numbering scheme for the fuel channels and Figure 5b shows the numbering of the fuel elements within each fuel channel. The fuel channels are numbered 1 through 16 (right to left, top to bottom), where each fuel channel contains six fuel elements/rods numbered 1 through 6 (from bottom to top). An “outer pin” is defined as a pin within fuel channels 1-4, 5, 8, 9, 12, 13-16. An “inner pin” is defined as a pin within fuel channels directly adjacent to the control rod (or fuel channels 6, 7, 10, 11). Results presented reference time step numbers (to determine the cumulative burnup associated with each time step refer to Table 4).

4	3	2	1
8	7	6	5
12	11	10	9
16	15	14	13

6
5
4
3
2
1

a. Radial

b. Axial

Figure 5. Numbering system of (a) fuel channels and (b) axial fuel pin/elements within fuel channels.

4.1. Prediction of k_{eff}

Figure 6 presents the predicted k_{eff} versus burnup for each method examined. The 1σ standard deviations are also included; however, because the standard deviations range from 0.00024 to 0.00031, the 1σ standard deviations are not visible. A successful iteration set is defined as predicting a k_{eff} critical to within 1σ standard deviation in 5 iterations or less. CATCE resulted in the largest amount of successful iteration steps throughout all 17 burn time steps. CATCE only encountered 2 cases – the 6th and 14th time step – where CATCE did not attain a successful iteration set. Over all burn time steps, the average k_{eff} predicted by CATCE was 1.00012 ± 0.00028 . As CATCE was the most successful method in predicting k_{eff} over all time steps, the CATCE method was used as the comparator for judging all other criticality search methods. MATCE mirrored the performance of CATCE, and the MATCE average predicted k_{eff} over all burn time steps was 1.00005 ± 0.00027 . MATCE, however, had twice the number of failed iterations (occurring on the 2nd, 5th, 6th and 14th time steps) compared to CATCE. Considering successful iterations alone, on average, MATCE took 0.36 less iterations per time step to converge when compared to CATCE (see Table 5). Considering both successful and failed iterations, on average,

MATCE took 0.17 less iterations than CATCE per time step to converge (see Table 5). In all failed iteration cases for both CATCE and MATCE, both methods would very likely have converged in the next iteration. However, increasing the maximum number of iterations allowed within the CRPE tool augments the computational expense, hence why the maximum number of iterations for the study was limited to five.

Table 5. CATCE and MATCE convergence.

*Criteria	Average number of iterations to converge	
	CATCE	MATCE
Success	4.00	3.64
Success & Failure	4.11	3.94

*Success = Convergence occurs in 5 iterations or less. *Failure = Convergence not attained in 5 iterations.

Figure 6. k_{eff} at various time steps for the different methods tested.

The next best accurate k_{eff} predictor, after CATCE and MATCE, was the PRE method. The PRE performed poorly in predicting k_{eff} , with an average prediction over all burn time steps being 0.99368 ± 0.00028 . In fact, the PRE only had one successful iteration set which occurred on the 14th time step. PRE consistently predicted subcritical k_{eff} s within the range 0.98 to 0.99. Of all methods tested in the CPRE tool, the LRE was the poorest, with an average k_{eff} prediction over all burn time steps being 0.97870 ± 0.00028 . Only a single successful iteration occurred during the 16th time step. For other LRE time steps, LRE struggled to come remotely close to critical, predicting mostly within the range of 0.96 to 0.97.

The hard coded critical position was the only time step in which the ICS method predicted k_{eff} to within a 1 σ standard deviation. In the absence of a robust criticality search routine in *Monteburns*, this

method is probably the manner in which most *Monteburns* users perform depletion calculations. As can be seen in Figure 6, it does not maintain a critical spectra throughout the depletion calculation.

The NCS method – in which predicting the critical position was not initiated – demonstrated the result of voiding the control rod position throughout the burnup. Initially, the reactor was supercritical due to the absence of a control rod. The subsequent time steps caused a reduction of the system k_{eff} due to the buildup of Sm-149 and Xe-135, both of which are strong neutron absorbers. When the production of these two isotopes reached equilibrium concentrations around the 4th and 5th time steps, Pu-239 breeding overcame the effect of fission product poisons, which actually added to the reactivity of the system. Eventually, Pu-239 production reached an equilibrium and fissile material depletion dominated.

4.2. Calculation Times

The calculation times for each tested method are shown in Table 6. The ICS had the least computational burden. The NCS method took longer than the ICS, as supercritical calculations take a longer time to complete than subcritical calculations in MCNP due to more fissions occurring and more neutrons remaining within the system (scattering down in energy) for a longer period of time. LRE and PRE both required about 16% more time than NCS. MATCE and CATCE both had the most computational burden, needing about 40% more time than NCS. Therefore implementing a more accurate method resulted in an increase in computational time.

Table 6. Percent increase in calculation times compared to ICS; percent increase = $100 \left| \left(\frac{A}{B} - 1 \right) \right|$ where B is the NCS calculation time and A is either the NCS, LRE, PRE, MATCE or CATCE calculation times.

Method	% increase in calculation times
ICS	0
NCS	96.1
LRE	128.2
PRE	128.6
MATCE	174.4
CATCE	182.1

4.3. Power Densities at Varying Time Steps

Presented in Figures 7-8 are axially dependent power profiles for varying time steps of the graphite reactor model. Each figure shows the axial power density profile (power per each of the 6 axial locations) for all “outer” and “inner” fuel pins in a fuel channel. An “inner” fuel pin is defined as being adjacent to the control rod. An “outer” fuel pin is defined as being further away from the control rod.

The NCS model, as expected, exhibited a cosine behavior axially due to the absence of the control rod in the geometry as well as uniform axial moderator and fuel temperature. The maximum power density occurred around the 3rd and 4th axial fuel pin location. The power density tapered off in the graphite region (not shown in Figure 7). The radial power density profile (not displayed) was “flat” due to the use of fully reflected boundary conditions in the x and y directions. The peak to average power ratio was 1.20 and 1.08 for the 2nd and 17th time steps. The peak to average power ratio was calculated by

taking the maximum power density for all six axial locations, and dividing by the average power density for all six axial locations. The ICS model exhibited a behavior consistent with LRE, PRE, CATCE and MATCE at the 2nd burn time step because of the presence of the control rod. However, at the 17th time step, the behavior was similar in nature to that of the NCS method.

The LRE, PRE, CATCE and MATCE methods exhibited different varying axial power profiles due to a number of factors: (1) continual change in the position of the control rod results in a change of absorption; (2) change in absorption affects the magnitude and spectra of the flux; (3) change in the magnitude and spectra of the flux changes the fission rate, which also affects the shape and spectra of the flux; (4) the shape and spectra of the flux will affect the buildup of fission products, actinides and neutron poisons and how these nuclides are distributed along the different axial locations.

At the 2nd time step (see Figure 7), the critical rod position was at 82.6% of the 5.4 m maximum control rod insertion length (see Figure 10). Since the rod was inserted from the top to the bottom, the cosine shape of the power density was perturbed. As such, the fuel pins at the top, on average, had a power density a factor of 6 lower than the average power density for all six axial locations (as seen in Figures 7 and 8) due to absorption of neutrons within the vicinity of the control rod. Consequently, the pins at the bottom had a power density of a factor of 3.5 higher than the average of all six axial locations. At the 2nd time step, the peak to average power ratio for LRE, PRE, CATCE and MATCE was 2.25, 2.16, 2.14 and 2.13. At the 17th burn time step, the peak to average power ratio for LRE, PRE, CATCE and MATCE was 1.79, 1.78, 1.75 and 1.76. The peak to average power density should have a temporal behavior and flatten with time, but this phenomenon was not evident for lower burnup.

At the 17th time step (see Figure 8), the critical rod position was at 15.9% of the maximum active rod length. Throughout the earlier burn time steps, the maximum power density was located at the bottom region. Consequently, at the 17th time step, the majority of the fissile material at the bottom end of the reactor had been depleted resulting in a greater amount of fissile material present at the fuel pins located in the upper region of the assembly. As a result, at the 17th time step, the maximum power density is located in the upper axial locations. Figures 9 and 10 show this in more detail, in that the peak of the flux was dictated by the position of the control rod. Continued withdrawal of the control rod resulted in a displacement of the peak of the flux from the lower axial fuel locations (at lower burnup) to the upper axial fuel locations (at higher burnup).

At the 2nd time step MATCE had a best case power density percent difference of -0.40% when compared to CATCE for all axial locations, as well as a worst case axial power density percent difference of -9.84% when compared to CATCE. For PRE, the best and worst case power density percent difference range was 0.74% and 9.43% for all axial locations. The LRE best and worst case percent differences were -6.64% and 60.76% for all axial locations. For the 17th time step, the best and worst case power density percent differences for MATCE was 0.00% and -3.78%, 0.00% and -4.03% for PRE, 1.41% and 15.33% for LRE for all axial locations.

★NCS △ICS ○LRE ×PRE +MATCE ◇CATCE

a. Outer pin

★NCS △ICS ○LRE ×PRE +MATCE ◇CATCE

b. Inner pin

Figure 7. Power density at 2nd burnup time step (0.017 GWD/MTU).

★NCS △ICS ○LRE ×PRE +MATCE ◇CATCE

a. Outer pin

★NCS △ICS ○LRE ×PRE +MATCE ◇CATCE

b. Inner pin

Figure 8. Power density at 17th burnup time step (8.0 GWD/MTU).

a. Outer pin

b. Inner pin

Figure 9. Evolution of CATCE power density at select burn time steps (8, 14, 15, 16, 17) corresponding to 0.6, 3.0, 4.5, 6.0, and 8.0 GWD/MTU of cumulative burnup.

Figure 10. Critical control rod positions for the different methods tested throughout burnup calculation relative to the length of fuel channel (containing six fuel elements stacked one on top of the other). The dotted line denotes the maximum distance the control rod is permitted to travel .

4.4. Bottom Fuel Pin (Axial Location 1)

Presented here are isotopic differences for an axial location at the bottom of the fuel channel between a pin near the control rod (“inner”) and a pin far from the control rod (“outer”) fuel pin. Numerical comparisons given in this section apply only beyond the 5th time step to give burn time for the buildup of lower yield minor actinides such as U-232, Pu-241 and Pu-242. Percent differences between the comparator (CATCE) and other methods tested within the CRPE tool are presented in an effort to determine which CRPE methodologies consistently match each other at isotopic predictions between the 5th (0.3 GWD/MTU) and 17th (8 GWD/MTU) time steps.

4.4.1. Uranium Isotopic differences

All methods were compared to CATCE. Percent difference plots for select uranium isotopes of interest are presented in Figures 11-17. The NCS method is excluded from the Figures because the percent differences associated with NCS in certain cases (see Figure 11) were very large and caused a distortion of the scale of the graphs. Table 7 shows, at axial location 1, the maximum percent differences in uranium isotopics compared to CATCE between the 5th and 17th burn time steps for all CRPE methodologies tested.

Table 7. Maximum percent difference in uranium isotopics compared to CATCE between the 5th and 17th time steps; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Isotope	Maximum percent difference compared to CATCE			
	ICS	LRE	PRE	MATCE
U-232	82.36	11.45	11.12	3.49
U-233	38.94	48.61	51.26	21.11
U-234	-9.33	-1.50	-0.95	0.95
U-235	32.70	-4.91	-2.52	-1.75
U-236	12.46	8.52	2.94	1.35
U-238	0.00	0.00	0.00	0.00

Between 0.3 GWD/MTU and 8 GWD/MTU for axial location 1, uranium isotope prediction (with the exception of U-233) compared to CATCE can be achieved to within 4% for MATCE, 12% for PRE and 12% for LRE. U-238 was accurately predicted without percent difference by all methods due to its large mass, and significant figures tracked in the output (see Figure 17). We subsequently excluded all U-238 percent difference plots from this point onwards, since other axial locations mirror this plot.

Table 7 gives credence to the fact that isotopic inventory is wildly different when burning with a critical spectrum than when burning without. This result was expected, and backed by section 4.3 in which a clear and distinct difference in the power densities was evident when burning with a critical spectrum versus without a critical spectrum at both beginning and end of life. The introduction of the control rod at a critical position throughout the depletion calculation and at different burn time steps perturbed the magnitude and shape of the flux; and the shape of the flux in turn drove the production of transuranic actinides.

a. Outer pin

b. Inner pin

Figure 11. Percent difference in U-232 compared to CATCE for an (a) outer pin location (b) inner pin location;
percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is NCS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 12. Percent difference in U-232 compared to CATCE for an (a) outer pin location and (b) inner pin location;
percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 13. Percent difference in U-233 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 14. Percent difference in U-234 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 15. Percent difference in U-235 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 16. Percent difference in U-236 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Figure 17. Percent difference in U-238 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

4.4.2. Plutonium Isotopic differences

As plutonium has resonances in thermal ranges, the shape of the thermal flux is critical to the buildup and depletion of Pu isotopes. For axial location 1, there is not much of a difference in the isotopics of an “outer pin” versus an “inner pin”. Figure 18 displays the neutron flux for the outer and inner fuel pins examined at the 5th and 15th burn time steps. As the thermal flux is similar for both outer and inner pin, the Pu isotopics is expected to follow the same trend in this axial location. Percent difference plots for select plutonium isotopes of interest are presented in Figures 19-23. Table 8 shows, at axial location 1, the maximum percent differences in plutonium isotopics compared to CATCE between the 5th and 17th burn time steps for all CRPE methodologies tested.

Table 8. Maximum percent difference in plutonium isotopics compared to CATCE between the 5th and 17th time steps; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Isotope	Maximum percent difference compared to CATCE			
	ICS	LRE	PRE	MATCE
Pu-238	82.87	19.64	4.92	4.92
Pu-239	10.90	8.53	2.75	0.91
Pu-240	-31.45	17.39	4.84	1.88
Pu-241	52.25	32.82	10.91	3.48
Pu-242	90.27	32.82	12.61	4.55

Between 0.3 GWD/MTU and 8 GWD/MTU for axial location 1, plutonium isotope prediction compared to MATCE can be achieved to within 5% for MATCE, and 13% for PRE. LRE is not reliable in this case as its maximum percent differences, relative to the methods that predict critical position well, are too significant.

a. Burn time step 5

b. Burn time step 15

Figure 18. Outer and inner pin neutron flux at thermal energies for (a) 5th burn time step (0.3 GWD/MTU) and (b) and 15th burn time step (4.5 GWD/MTU) .

a. Outer pin

b. Inner pin

Figure 19. Percent difference in Pu-238 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 20. Percent difference in Pu-239 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 21. Percent difference in Pu-240 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 22. Percent difference in Pu-241 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 23. Percent difference in Pu-242 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

4.5. Middle Fuel Pin (Axial Location 4)

Presented here are isotopic differences for an axial location in the middle of the fuel channel between a pin near the control rod (“inner”) and another pin away from the control rod (“outer”) fuel pin. Numerical comparisons given in this section apply only beyond the 5th time step to give burn time for the buildup of lower yield minor actinides such as U-232, Pu-241 and Pu-242. Percent differences between the comparator (CATCE) and other methods tested within the CRPE tool are presented in an effort to determine which CRPE methodologies consistently match each other at isotopic predictions between the 5th (0.3 GWD/MTU) and 17th (8 GWD/MTU) time steps.

4.5.1. Uranium Isotopic differences

Percent difference plots for select uranium isotopes of interest are presented in Figures 24-28. The percent difference plot for U-238 is excluded since it mirrors Figure 17. Table 9 shows, at axial location 4, the maximum percent differences in uranium isotopics compared to CATCE between the 5th and 17th burn time steps for all CRPE methodologies tested.

Table 9. Maximum percent difference in uranium isotopics compared to CATCE between the 5th and 17th time steps; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Isotope	Maximum percent difference compared to CATCE			
	ICS	LRE	PRE	MATCE
U-232	27.70	40.38	7.04	-3.31
U-233	77.73	114.29	-37.90	41.60
U-234	4.55	0.99	1.08	0.90
U-235	-23.44	-3.33	1.56	0.78
U-236	-8.42	29.14	5.29	-1.95
U-238	0.80	0.00	0.00	0.00

Between 0.3 GWD/MTU and 8 GWD/MTU for axial location 1, uranium isotope prediction (with the exception of U-233) compared to CATCE can be achieved to within 4% for MATCE, and 8% for PRE.

a. Outer pin

b. Inner pin

Figure 24. Percent difference in U-232 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 25. Percent difference in U-233 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 26. Percent difference in U-234 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 27. Percent difference in U-235 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Figure 28. Percent difference in U-236 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

4.5.2. Plutonium Isotopic differences

Again, due to the presence of resonances in thermal ranges of plutonium, the shape of the thermal flux is critical in driving the production of Pu isotopes. In axial location 1 (see section 4.4.2) the differences in neutron lethargy for “outer” and “inner” pins were marginal. This statement did not hold true for axial location 4. The maximum flux seen by the outer fuel pin (in axial location 4) was a factor of 4 less when compared to an outer fuel pin in axial location 1. In addition, the inner pin at axial location 4 experienced a 50% reduced neutron flux compared to an outer pin in axial location 4. The change in flux was due to the presence of the control rod as the inner pin in axial location 4 was within the active range of the control rod. As a result, the neutron flux for the inner and outer pin (in axial location 4) were dissimilar as confirmed in Figure 29. What is also distinct in Figure 29, is that the peak of the lethargy occurs around 10^{-7} MeV. Pu-239 has a resonance at this range; therefore the differences in isotopic buildup in axial location 4, for an inner pin versus an outer pin, was mainly driven by the difference in the neutron flux at the 10^{-7} MeV resonance.

Percent difference plots for select plutonium isotopes of interest are presented in Figures 30-34. Table 10 shows, at axial location 4, the maximum percent differences in plutonium isotopics compared to CATCE between the 5th and 17th burn time steps for all CRPE methodologies tested.

Table 10. Maximum percent difference in plutonium isotopics compared to CATCE between the 5th and 17th time steps; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Isotope	Maximum percent difference compared to CATCE			
	ICS	LRE	PRE	MATCE
Pu-238	-22.99	86.01	8.63	-6.42
Pu-239	4.52	25.99	4.82	-1.30
Pu-240	-17.68	63.88	11.72	4.35
Pu-241	17.97	95.35	12.99	-13.29
Pu-242	-34.03	163.55	17.03	-12.72

Between 0.3 GWD/MTU and 8 GWD/MTU for axial location 4, plutonium isotope prediction (with the exception of Pu-241 and Pu-242) compared to CATCE can be achieved to within 7% for MATCE. The trend, as one moves up along the fuel channel (approaching the active range of the control rod), seems to be a decrease in ability to predict plutonium isotopics for the CRPE methods that are poor predictors of critical rod position.

Figure 29. Outer and inner pin neutron flux at thermal energies for (a) 5th burn time step (0.3 GWD/MTU) and (b) and 15th burn time step (4.5 GWD/MTU) .

a. Outer pin

b. Inner pin

Figure 30. Percent difference in Pu-238 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 31. Percent difference in Pu-239 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 32. Percent difference in Pu-240 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 33. Percent difference in Pu-241 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Figure 34. Percent difference in Pu-242 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

4.6. Top Fuel Pin (Axial Location 6)

Presented here are isotopic differences for an axial location at the top of the fuel channel between a pin near the control rod (“inner”) and a pin far from the control rod (“outer”) fuel pin. Numerical comparisons given in this section apply only beyond the 5th time step to give burn time for the buildup of lower yield minor actinides such as U-232, Pu-241 and Pu-242. Percent differences between the comparator (CATCE) and other methods tested within the CRPE tool are presented in an effort to determine which CRPE methodologies consistently match each other at isotopic predictions between the 5th (0.3 GWD/MTU) and 17th (8 GWD/MTU) time steps.

4.6.1. Uranium Isotopic differences

Percent difference plots for select uranium isotopes of interest are presented in Figures 35-39. The percent difference plot for U-238 is excluded since it mirrors Figure 17. Table 11 shows, at axial location 6, the maximum percent differences in uranium isotopics compared to CATCE between the 5th and 17th burn time steps for all CRPE methodologies tested.

Table 11. Maximum percent difference in uranium isotopics compared to CATCE between the 5th and 17th time steps; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Isotope	Maximum percent difference compared to CATCE			
	ICS	LRE	PRE	MATCE
U-232	93.89	116.18	58.42	-6.65
U-233	185.71	-95.12	-58.50	-63.38
U-234	-3.55	-1.67	0.30	0.34
U-235	-14.98	-4.80	-0.40	0.85
U-236	56.42	88.29	15.85	-7.40
U-238	0.00	0.00	0.00	0.00

Between 0.3 GWD/MTU and 8 GWD/MTU for axial location 6, uranium isotope prediction (with the exception of U-233) compared to CATCE can be achieved to within 8% for MATCE. PRE is only reliable in this axial location for predicting U-234, U-235 and U-238.

Figure 35. Percent difference in U-232 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Figure 36. Percent difference in U-233 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

△ICS ○LRE ×PRE +MATCE

a. Outer pin

△ICS ○LRE ×PRE +MATCE

b. Inner pin

Figure 37. Percent difference in U-234 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

△ICS ○LRE ×PRE +MATCE

a. Outer pin

△ICS ○LRE ×PRE +MATCE

b. Inner pin

Figure 38. Percent difference in U-235 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

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688 Figure 39. Percent difference in U-236 compared to CATCE for an (a) outer pin location and (b) inner pin location;
 689 percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

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692 4.6.2. Plutonium Isotopic differences

693 The neutron flux behavior seen in axial location 4 (section 4.5.2) was expected to be replicated in axial
 694 location 6 as both axial locations are within the active range of the control rod. Figure 40 confirms this,
 695 although the peak values for flux are different. The maximum flux in axial location 6 (top fuel pin) is
 696 about 0.75 order of magnitude less than that of axial location 4 (middle fuel pin), and 1.4 order of
 697 magnitude difference from axial location 1 (bottom fuel pin). Akin to axial location 4, the differences in
 698 isotopic buildup at axial location 6, for an inner pin versus an outer pin, will be driven by the difference
 699 in the lethargy at the 10^{-7} MeV resonance. Percent difference plots for select plutonium isotopes of
 700 interest are presented in Figures 41-45. Table 12 shows, at axial location 6, the maximum percent
 701 differences in uranium isotopics compared to CATCE between the 5th and 17th burn time steps for all
 702 CRPE methodologies tested.

703 Table 12. Maximum percent difference in plutonium isotopics compared to CATCE between the 5th and 17th time
 704 steps; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

Isotope	Maximum percent difference compared to CATCE			
	ICS	LRE	PRE	MATCE
Pu-238	224.62	271.13	29.90	-29.84
Pu-239	48.89	86.32	15.78	-7.99
Pu-240	124.11	257.08	34.76	-14.56
Pu-241	326.15	462.50	64.45	-30.25
Pu-242	578.45	967.90	82.08	-31.28

Between 0.3 GWD/MTU and 8 GWD/MTU for axial location 6, MATCE can only predict Pu-239 compared to CATCE to within 8%. The other methods struggle at this axial location. The best explanation for this is that throughout the burnup calculation, this axial region sees a compression of the flux by the control rod. As such, the presence of the control rod suppresses the predictability of isotopics at this axial location because the accuracy of critical rod position prediction affects how much of the fuel within the axial location is exposed to neutrons for fission events.

Figure 40. Outer and inner pin neutron flux at thermal energies for (a) 5th burn time step (0.3 GWD/MTU) and (b) and 15th burn time step (4.5 GWD/MTU) .

Figure 41. Percent difference in Pu-238 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

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Figure 42. Percent difference in Pu-239 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

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Figure 43. Percent difference in Pu-240 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

730

a. Outer pin

b. Inner pin

Figure 44. Percent difference in Pu-241 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

a. Outer pin

b. Inner pin

Figure 45. Percent difference in Pu-242 compared to CATCE for an (a) outer pin location and (b) inner pin location; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is ICS, LRE, PRE and MATCE.

4.7. 8 GWD/MTU Isotopic differences

In sections 4.4 to 4.6, the results for the isotopic differences at three different locations were presented, and maximum percent differences were examined through the burn time steps. However, certain isotopes proved difficult to predict between the 5th and 17th time step. For example, at axial location 6 on the 9th time step, there was a -30.25% percent difference for Pu-241 when MATCE was compared to CATCE. At the 13th time step, this percent difference reduced to -8.15%, and at the 15th time step percent difference was 3.87%. At the 16th time step, the percent difference was -20.00%, and at the 17th (or final time step), the percent difference was 0.75%.

This oscillating trend of percent differences was persistent throughout all axial locations for U-233, Pu-241 and Pu-242, and was most pronounced as one approached the upper axial locations of the fuel channel. The trend of the magnitude of oscillation was even greater for PRE, LRE, NCS, and ICS. As a result, for any CRPE estimation method, there was no consistent percent difference trend through all burn time steps for U-233, Pu-241 and Pu-242. The reason for this oscillating trend was that overshooting depletion at one time step (due to overshooting fission rate) resulted in more fission product poison being developed at the next time step. More fission product poison at the next time step resulted in lower fission rate relative to absorption undershooting burnup. The integral result is that the burnup can oscillate from overshoot to undershoot dampening about the average. In addition, isotopes like Pu-241 and Pu-242 were dependent on Pu-240 presence. Therefore without equilibration of Pu-240 in the system, the production and prediction of Pu-241 and Pu-242 were adversely affected. Table 13 shows the percent difference in isotopics for all methods compared to CATCE and at three different axial locations at 8 GWD/MTU. The table displays only the inner pins, as the earlier section determined these were harder to predict due to the active control rod presence at axial locations 4 and 6.

Table 13. Percent difference in uranium isotopic inventory, as compared to CATCE for select axial locations; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is NCS, LRE, PRE and MATCE.

Axial Location	% Difference in isotopics at 8 GWD/MTU compared to CATCE						
	Method	92232	92233	92234	92235	92236	92238
1 (Bottom Fuel Pin)	NCS	19.88	-30.63	6.31	37.26	-14.60	0.00
	ICS	82.36	3.34	-9.33	-32.70	12.46	0.00
	LRE	6.83	2.70	-0.96	-3.42	1.42	0.00
	PRE	1.00	-2.70	-0.19	-1.90	0.71	0.00
	MATCE	1.00	-1.50	-0.76	-0.76	0.41	0.00
4 (Middle Fuel Pin)	NCS	-22.65	18.92	-2.71	-11.43	4.23	0.00
	ICS	-24.17	1.85	4.55	23.44	-8.41	0.00
	LRE	-4.27	8.56	-0.19	1.43	-0.72	0.00
	PRE	-0.85	18.02	-0.39	0.36	-0.21	0.00
	MATCE	-1.71	12.16	-1.16	1.07	-0.62	0.00
6 (Top Fuel Pin)	NCS	32.56	80.27	-9.54	-35.66	50.17	-0.79
	ICS	14.81	15.33	-1.84	-9.60	12.01	0.00
	LRE	14.08	-4.08	-1.48	-5.70	7.52	0.00
	PRE	0.84	-29.93	-0.66	-0.74	0.52	0.00
	MATCE	2.73	-27.21	-0.49	-0.18	-0.17	0.00

Table 13 shows the inaccuracy of NCS in predicting the isotopics at 8 GWD/MTU, as it only predicted U-238 isotopics consistently. The maximum percent differences at axial locations 1, 4 and 6 for all uranium isotopes examined were 37.26%, -22.65% and 50.17%. The ICS maximum percent differences at axial locations 1, 4 and 6 for all uranium isotopes examined were 82.36%, -24.17% and 15.33%. The LRE maximum percent differences at axial locations 1, 4 and 6 for all uranium isotopes examined were 6.83%, 8.56% and 14.08%. For all uranium isotopes examined, PRE yielded maximum percent differences at axial locations 1, 4 and 6 of 2.70%, 18.02% and -29.93%, while for MATCE, the maximum percent differences for all uranium isotopes were -1.50%, 12.16% and -27.21%. These results prove MATCE to be the best predictor for 8 GWD/MTU isotopics compared to CATCE, seconded by PRE. Anomalies occur at certain 8 GWD/MTU predictions, for example, in axial location 4 for U-233 where LRE outperforms PRE and MATCE. This is attributed mostly to statistical fluctuation of the flux calculation and propagation of the atom density error.

Table 14. Percent difference in plutonium isotopic inventory, as compared to CATCE for select axial locations; percent difference = $100 \left(\frac{A}{B} - 1 \right)$ where B is CATCE and A is NCS, LRE, PRE and MATCE.

		% Difference in isotopics at 8 GWD/MTU compared to CATCE				
Axial Location	Method	94238	94239	94240	94241	94242
1 (Bottom Fuel Pin)	NCS	-52.98	-7.59	-28.3	-23.16	-54.2
	ICS	82.86	3.81	31.45	52.25	90.27
	LRE	6.32	-0.32	3.14	4.91	9.82
	PRE	2.81	-0.63	2.52	2.11	4.46
	MATCE	0.00	0.00	1.89	0.00	1.79
4 (Middle Fuel Pin)	NCS	41.52	1.27	9.74	1.69	14.04
	ICS	-22.99	-1.26	-17.74	-17.74	-34.03
	LRE	2.23	0.00	-0.65	-4.78	-4.39
	PRE	0.45	0.95	-1.3	-1.97	-1.75
	MATCE	0.00	0.63	-0.65	-3.93	-3.51
6 (Top Fuel Pin)	NCS	552.36	24.89	126.67	112.96	379.34
	ICS	75.27	8.91	27.56	23.48	55.06
	LRE	33.48	5.06	15.43	26.85	42.15
	PRE	1.72	-0.42	1.14	1.85	4.96
	MATCE	-6.01	0.00	0.76	0.00	-1.65

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Table 14 shows the inaccuracy of NCS, again, in predicting the isotopics at 8 GWD/MTU for plutonium isotopes, with maximum percent differences at axial locations 1, 4 and 6 for all plutonium isotopes examined at -52.98%, 41.52% and 552.36%. The ICS maximum percent differences at axial locations 1, 4 and 6 for all plutonium isotopes examined yielded values of 90.27%, -34.03% and 75.27%. The LRE maximum percent differences at axial locations 1, 4 and 6 for all plutonium isotopes examined yielded values of 9.82%, -4.39% and 42.15%. For all plutonium isotopes examined, PRE yielded maximum percent differences at axial locations 1, 4 and 6 of 4.46%, -1.75% and 4.96%, while for MATCE, the

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maximum percent differences for plutonium isotopes were 1.89%, -3.93% and -6.01%. These results, again, prove MATCE to be the best predictor for 8 GWD/MTU isotopics when compared to CATCE.

5. Conclusion

This paper has presented a control rod position estimator (CRPE) tool that was developed within *Monteburns* for the purpose of maintaining a critical spectra through a depletion calculation with the use of a control rod. Four methods of estimating critical position were incorporated within the CRPE tool. Two methods (named CATCE and MATCE) employed an inverse multiplication methodology, one method (named PRE) used a polynomial fit methodology and the final method (named LRE) used a linear fit methodology.

The MATCE and CATCE methods predicted similar temporal k_{eff} s, power densities, and isotopic inventory of transuranic actinides. At axial location 1 (bottom fuel channel), which was outside the active movement range of the control rod, MATCE predicted to within 1%, all 8 GWD/MTU plutonium isotopics similar to CATCE (with the exception of Pu-240 and Pu-242). At axial location 4 (corresponding to the middle of the fuel channel which was within the active range of the control rod), MATCE's prediction at 8 GWD/MTU was within 0.65% of CATCE for all plutonium isotopes tracked (with the exception of Pu-241 and Pu-242). At axial location 6 (corresponding to the top of the fuel channel which was also within the active range of the control rod), MATCE's predicted CATCE within 2%, at 8 GWD/MTU, for all plutonium isotopes tracked (with the exception of Pu-238). Given MATCE and CATCE's consistence in prediction, either method would be recommended as suitable for performing a fuel depletion calculation.

The PRE method, though a bad predictor of k_{eff} , performed surprisingly well in predicting power densities and 8 GWD/MTU isotopics. At axial location 1 which was outside the active movement range of the control rod, PRE predicted all 8 GWD/MTU plutonium isotopics to within 3% (with the exception of Pu-242). At axial location 4 (within the active range of the control rod), the accuracy in prediction at 8 GWD/MTU was within 2% for all Pu isotopes tracked. At axial location 6 (also within the active range of the control rod), the accuracy in prediction was within 2% for all plutonium isotopes tracked (with the exception of Pu-242). Given the reduced computational calculation time involved with a PRE calculation and its 8 GWD/MTU plutonium isotopics predictions relative to CATCE, the PRE method is considered a viable alternative to CATCE and MATCE. Earlier, the authors chose their definition of a successful critical iteration to be $k_{eff} = 1.0$ within a standard deviation. The 8 GWD/MTU plutonium isotopics prediction of PRE may hint that this strict definition of a critical iteration may be unnecessary. PRE's k_{eff} values (which ranged largely between 0.98 and 1.0 throughout all burn time steps) were sufficient enough to predict 8 GWD/MTU plutonium isotopics largely consistent with that of CATCE and MATCE.

The LRE, ICS, and NCS are not recommended for use in any type of fuel depletion calculation. The poor k_{eff} prediction, and percent differences posited for power density estimation, and isotopic inventory when compared to CATCE are too significant to ignore. One should also note here that LRE had k_{eff} predictions that ranged from 0.96 to 1, while k_{eff} values using the ICS method ranged from 0.91 to 1. As such, dropping below PRE's worst k_{eff} predictions (a threshold value of 0.98) led to an inability to predict 8 GWD/MTU plutonium isotopics consistent with that of CATCE and MATCE. NCS on the other hand had consistently supercritical k_{eff} predictions resulting in wildly different isotopic predictions compared to CATCE and MATCE. A noticeable trend for LRE, ICS, and NCS is that the 8 GWD/MTU isotopic predictions get worse as one approaches the active range of the control rod.

The percent differences in the results section do not reflect the propagation of the percent difference of the atom density (from the Monte Carlo fission rate calculations) as a function burnup as *Monteburns* does not currently propagate these percent differences. Slight changes in atom density can affect the shape of the thermal Maxwellian distribution and perturb the energy dependent flux in and out of thermal resonances. Generally speaking, for uranium isotopes low energy resonances tend to be greater than 1 eV; and therefore slight shifts in the stochastic behavior of the atom density propagation were thought not to affect the direct transmutation of these nuclides (the exception is the production from decay of plutonium isotopes). Nonetheless, once a percent difference propagation scheme is placed within *Monteburns*, the isotopic differences should be reexamined to determine if the percent differences are statistically different. Future studies should also examine the amount of iterations required for MATCE and CATCE to meet a converged critical position and the computational cost of extending the allowed iterations. The authors also note that the major assumption presented here is that criticality is maintained only by perturbing available geometry in the truncated model.

This study only examined the effect of one control rod on isotopic inventory. A graphite moderated gas cooled reactors can have in excess of 45 active control rods. Maintaining a critical spectra in a real life scenario would require manipulation of many control rods at the same time, with the control rods at varying axial heights. In reality, interface leakage of surrounding fuel arrays also influence criticality. At the time of this study, an energy dependent albedo capability was not available in a released version of MCNP6 [37]. Future studies should asses the use of other criticality preservation techniques during the burnup for truncated geometries; nonetheless, the work here does demonstrate the effectiveness of the presented techniques for maintaining criticality during burnup and the consequence on isotope prediction.

While currently, the CRPE tool can only search for estimated critical position for a single control rod, future developmental work could be geared toward implementing additional features, such as the ability to change the heights of a group of control rods or the introduction of neutron poisons such as boric acid, at arbitrary time steps in the calculation to simulate shut down and/or reactor scram scenarios.

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