ORIGEN-S Decay Heat Calculations from NuFLASH and SORO Detailed Bundle Data

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ABSTRACT

Title: **ORIGEN-S Decay Heat Calculations from NuFLASH and SORO Detailed Bundle Data**
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Abstract

As part of the Nuclear Waste Management Organization's (NWMO) program to investigate the integrity of used nuclear fuel, the temperature of an instrumented Dry Storage Container (DSC) DSC-812, loaded with 384 CANDU fuel bundles, was monitored at the Western Waste Management Facility (WWMF) starting in September 2007. The NWMO requires key data including used fuel burn-up and heat of decay (thermal output) for each of the fuel bundles stored in the DSC including their location within the storage modules and the DSC. This information will form part of a planned subsequent study to complete a thermal analysis of DSC-812.

The decay heat for 22 selected bundles (representing all 384 bundles in DSC-812) was calculated with ORIGEN-S using bundle data extracted from the NuFLASH fuel accounting database and the SORO production physics database. It was found that the ORIGEN-S decay heat for the 22 subject bundles, calculated at cooling times of 10 years or longer, was independent of specific bundle power histories, and could be predicted strictly from the specific bundle burn-up assuming a typical (core average) bundle power. An upper bound to the 1-sigma uncertainty in the predicted decay heat values at relevant decay times is estimated to be 10%. The report provides the methodology, key calculations, and results.

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1. INTRODUCTION

As part of the Nuclear Waste Management Organization's (NWMO) program to investigate the integrity of used nuclear fuel, the temperature of an instrumented Dry Storage Container (DSC) DSC-812, loaded with 384 CANDU fuel bundles, is currently being monitored at the Western Waste Management Facility (WWMF). NWMO requires key data including used fuel burn-up and heat of decay (thermal output) for each of the fuel bundles stored in the DSC including their location within the storage modules and the DSC. This information will form part of a planned subsequent study to complete a thermal analysis of DSC-812.

2. OBJECTIVE

The main objective of this work was to calculate decay heat power for 22 representative bundles (out of 384 in total) in DSC-812 at two specific times:

1) 10 years after discharge from the reactor core; and

2) As of September 30th, 2007.

The decay heat power calculations were performed using the ORIGEN-S SCALE 4.2 (Hermann and Westfall, 1995) code. In addition, an estimate of the uncertainty in the decay heat calculations and an examination of the sensitivity of decay heat to bundle power history was required.

3. BACKGROUND

Temperature readings, obtained with thermocouples imbedded in the inner and outer skin of the DSC wall, form a part of the data required to analyze the DSC thermal performance. Another component of the data required for thermal performance analysis consists of heat of decay (thermal output) associated with each of the bundles.

DSC-812 was loaded by Bruce Power with 384 37-element NU fuel bundles from the Bruce B station, and a record of key spent fuel data was provided to OPG, who operate the WWMF. The key spent fuel data includes:

1) Bundle serial number;

2) Bundle type (for initial U-235 isotopic value);

3) Bundle power history (including loading date, discharge date, and location in the core);

4) Bundle burn-up (energy production);

5) Bundle mass; and

6) Bundle location in the DSC.

The decay heat for the entire DSC will be determined from calculations using 22 representative bundles chosen by NWMO. This approach was used to reduce the effort that would otherwise have been required to prepare detailed power histories for each of the 384 bundles in the DSC. Examination of the sensitivity of decay heat to bundle power history is included in this report to confirm the effectiveness of the approach.

4. METHODOLOGY

The procedure used to calculate decay heat powers for each of the specified fuel bundles was as follows:

1) Retrieve bundle data from the NuFLASH (Nuclear Fuel Location and Storage History) (Walmsley, 2003) system;

2) Retrieve bundle power histories from the production SORO (Simulation of Reactor Operation) database (Gifford, 2004) using the BNDHST (Johnston, 2005) utility;

3) Simplify the bundle power histories to block averages;

4) Calculate the isotope masses in bundles prior to irradiation;

5) Calculate the cooling time from discharge to September 30, 2007;

6) Prepare the ORIGEN-S input data files;

7) Calculate decay power at 10 years and at September 30, 2007 with ORIGEN-S;

8) Prepare a reference curve by plotting decay heat at 10 years cooling time versus discharge burn-up for a constant core average bundle power;

9) Compare the ORIGEN-S calculated decay heat values at 10 years with the reference curve; and

10) Perform an assessment of the uncertainty in the ORIGEN-S decay heat calculations.

Each of these steps is further explained in the following subsections.

4.1 BUNDLE DATA

The 22 bundle IDs specified by NWMO (Table 1) are as follows:

L90964C, K23334Z, K13749Z, K37331Z, K23722Z, K23683Z, K11377Z, K36759Z, K11339Z, K36419Z, K07950Z, K08380Z, K08307Z, L77222C, K27259Z, K07258Z, L90248C, Q00877C, L94448C, L82133C, L90687C, and K26434Z.

The bundle serial number, bundle type, bundle location within the DSC[1], discharge date, and bundle specific Uranium mass was retrieved from the NuFLASH fuel accounting system for each of the 22 bundles specified.

4.2 BUNDLE POWER HISTORIES

Bundle discharge locations and dates retrieved from NuFLASH were used to retrieve the power histories for each of the 22 specified bundles from the production SORO database using the SORO utility BNDHST. The bundle power histories were copied to MS Excel for further processing and simplification to block average power histories.

4.3 SIMPLIFIED BUNDLE POWER HISTORIES

The bundle power histories retrieved from the production SORO database are bundle thermal powers at specific bundle burn-ups. These were then converted in MS Excel spreadsheets into bundle fission power versus cumulative dwell time using the following formulae.

$$DT_i = \frac{(BB_i - BB_{i-1}) \times BM}{BP^f{}_{i-1} \times 24(h/day)}$$

And:

$$BP^f = BP^{th} / TFR$$

DT_i = i^{th} Dwell Time (days)

(Cumulative DT_i is $\sum_1^i DT_i$)

BB_i = SORO Bundle Burn-up at end of i^{th} Dwell Time (MWh/kgU)

BM = SORO Bundle Uranium Mass, 19.2126 kgU

BP^f = Bundle fission power (MW(f))

BP^{th} = Bundle thermal power (MW(th))

TFR = Thermal to Fission Ratio = 0.95441550

There were too many individual dwell steps to process practically with ORIGEN-S so the bundle power histories were plotted and then grouped into blocks of similar bundle powers. The groupings were somewhat arbitrary but captured periods of similar bundle fission powers. Such periods frequently occur when a bundle remains in a specific location with a similar reactor power. An average bundle fission power was determined for each block. See Figures 2 to 23 for specific plots of bundle fission power as a function of cumulative dwell time with corresponding block average bundle powers. These blocks of fission powers and dwell times were used in ORIGEN-S to calculate decay heat. Note that reactor power outages prior to discharge are not included in these calculations as these are typically small relative to the overall cooling period and cannot be extracted using BNDHST.

[1] Although NuFLASH contains accurate rack positions at BNGS-B, fuel handling staff does not have procedures in place to prevent the rotation of racks and trays prior to module loading. Since each tray is loaded into two rows within a module, bundle position accuracy may be limited to knowing that the bundle is in one of two rows (e.g. if bundle is slot H11 (flare end), it may actually be anywhere in rows G or H (12 bundle positions total).

4.4 BUNDLE SPECIFIC ISOTOPE MASS

Bundle specific U238, U235, and U234 isotope masses (g) were calculated using the bundle specific uranium masses from NuFLASH, and the U238, U235, and U234 isotope fractions from the ORIGEN-S reference abundances.

4.5 COOLING TIMES

The cooling times from discharge to September 30, 2007 were calculated for the 22 specified bundles (Table 2, Column 7). The cooling time for 10 years following discharge is the same for each bundle, namely 3650 days.

4.6 PREPARATION OF THE ORIGEN-S INPUT DATA FILES

The simplified bundle power histories (dwell time, bundle fission power), uranium isotope masses (g), and the cooling times (years) were used to generate the ORIGEN-S input files.

4.7 CALCULATION OF DECAY POWER

Decay powers at cooling times of 10 years and as of September 30, 2007 were calculated using ORIGEN-S.

4.8 CALCULATION OF THE REFERENCE CURVE

A reference curve (Figure 1) was prepared by plotting decay heat at 10 years following discharge versus bundle burn-ups ranging from 120 MWh/kgU to 260 MWh/kgU on the basis of a constant core average bundle power of 453.85 kW.

4.9 COMPARISON WITH THE REFERENCE CURVE

An examination of the sensitivity of decay heat to bundle power history was performed by comparing the decay powers at 10 years following discharge with the reference curve based on a core average bundle power.

4.10 ASSESSMENT OF THE UNCERTAINTY IN THE DECAY HEAT CALCULATIONS

An assessment of the uncertainty in the decay heat calculations was performed based on experimental and code-to-code comparisons for ORIGEN-S, and related uncertainty analysis for bundle discharge burn-up and reactor power.

5. COMPUTER CODES USED

Several computer codes were used in the calculations including NuFLASH, SORO, BNDHST, and ORIGEN-S. Other calculations were performed using MS Excel or MATLAB.

5.1 NuFLASH VERSION 20070301

NuFLASH is approved for use in this analysis (Schneider, 2009).

5.2 SORO VERSION 20060330

SORO (Simulation of Reactor Operation) and SORO utilities are approved for use in this analysis (Schneider, 2009).

5.2.1 BNDHST Version 2.0

BNDHST, a SORO utility used for extracting bundle history data, is approved for use in this analysis (Schneider, 2009).

5.2.2 ORIGEN-S Version 4.2

ORIGEN-S and its CANDU fuel libraries have been fully qualified for safety related analyses. This is embodied in the Tool Qualification Report (Albasha and Backham, 2001) and the corresponding Validation Manual (Backham and Albasha, 2001). The version of ORIGEN-S employed for this current analysis is SCALE 4.2.

6. RESULTS AND DISCUSSION

6.1 NuFLASH DATA FOR THE 22 SPECIFIED BUNDLES

The NuFLASH data extracted for the 22 specified bundles is summarized in Table 1.

6.2 SIMPLIFIED BUNDLE POWER HISTORIES

The simplified bundle power histories for the 22 bundles are illustrated in Figure 2 to Figure 23.

6.3 ORIGEN-S DECAY POWERS AT 10 YEARS COOLING TIME AND AT SEPTEMBER 2007

The ORIGEN-S calculated decay powers at 10 years cooling time and at September 30, 2007 are summarized in Table 2.

6.4 ORIGEN-S DECAY POWER AT 10 YEARS COOLING TME COMPARED WITH THE REFERENCE CURVE

The decay heat at 10 years cooling time calculated by ORIGEN-S is compared with the reference curve. The results show that decay heat is predominantly dependent on burn-up and independent of the power history as illustrated in Figure 24.

6.5 UNCERTAINTY IN THE DECAY HEAT CALCULATIONS

6.5.1 Assessment of ORIGEN-S Accuracy for Decay Heat Predictions

Two assessments of ORIGEN-S accuracy for decay heat predictions have been completed in the past. The first one (Albasha and Fredette, 2001) performed in 2001 as part of the ORIGEN-S SCALE 4.2 validation exercise, was done on the basis of experimental data for seventeen 19-element CANDU fuel bundles and concerned cooling times in the range of a few weeks to approximately 6 years. The 1-sigma uncertainty inferred in that work was 8.5%. In 2007 this assessment was revisited (Inglot and Morrison, 2007) and it was concluded that exclusion of selected questionable data points lead to a reduction of the 1-sigma uncertainty from 8.5% to 4.1%.

The second accuracy assessment (Inglot, 2008), completed in 2008, was focused on a cooling time range of 1 second to approximately 3 years and was done specifically for 28- and 37-element CANDU fuel. Due to a lack of experimental measurements of decay heat in this cooling time range, this assessment was performed on the basis of a code-to-code comparison.

The calculations used as surrogate for experimental data were based on the ANS-5.1 Standard formulation (ANSI/ANS-5.1-1994) as adapted to 28- and 37-element NU fuel. The 1-sigma uncertainty assessed in (Inglot, 2008) was 2.0%.

Since the previous two accuracy assessments did not cover the decay time range of interest here, namely, 10 to 15 years, an approximate upper-bound 1-sigma uncertainty has been inferred as part of this work. This assessment is based on estimating upper limits on the 1-sigma uncertainties for the two main components of decay heat power, namely, decay heat due to fission products and due to actinides, separately, and then combining them. The assessment of uncertainty associated with the fission product component is similar in nature to the previous accuracy assessment carried out in (Inglot, 2008), in that the ANS-5.1 Standard calculations of decay heat are used as a surrogate for experimental data. Based on a fuel burn-up range of 120 MWh/kgU to 260 MWh/kgU and a cooling time range of 10 to 15 years, the upper-bound limit on the uncertainty of that component is very conservatively[2] assessed at 6%. Due to a lack of appropriate validation data for actinide decay heat, however, the upper-bound 1-sigma uncertainty for this component is taken as 25%. This value is estimated based on the ORIGEN-S expected uncertainty on the inventory predictions for heavy elements with highest contributions to decay heat. The limits on the 1-sigma uncertainties for the two components are then combined assuming a maximum actinide contribution to total decay heat of 16%; this occurs for the burn-up 260 MWh/kgU and decay time of 15 years. The combined upper-bound 1-sigma uncertainty is then estimated to range[3] between 6.4% and 9.0%.

6.5.2 Assessment of the Uncertainty in Discharge Burn-up

There is no accepted reference for individual bundle discharge burn-up uncertainty. However, there are references for average bundle burn-up uncertainty and it was determined that the average uncertainty is largely due to reactor power uncertainty. An uncertainty of 1% was applied to reactor power in (Xie, 2007), and a 0.76% uncertainty was applied in (Seager, 2009). Therefore, 1% is a reasonable estimate of uncertainty to apply to the burn-up value input to the ORIGEN-S calculated decay heat. This assumes that the 22 bundles specified in this assessment are representative of typical discharged bundles.

6.5.3 Sensitivity of Decay Heat to Discharge Burn-up

Based on the reference curve, a 1% increase in discharge burn-up from 150 to 151.5 MWh/kgU results in a ~ 0.94% increase in decay heat from 3.66 to 3.69 W at 10 years. For a bundle with higher discharge burn-up, a 1% increase in discharge burn-up from 250 to 252.5 MWh/kgU results in a 0.96% increase in decay heat from 5.95 to 6.00W at 10 years.

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[2] The conservative nature of this estimate stems from the fact that the inherent (upper-bound) uncertainty in the ANS-5.1 Standard decay heat predictions (~4%) and the difference between the best-estimate ANS and ORIGEN-S calculations (2%) are added linearly. Inspection of the underpinning data indicates that the ORIGEN-S predictions (for the range of burn-ups inspected in this work) always fall within the range provided by the 1-sigma random uncertainties from the ANS Standard, and their distribution is rather random. As such, a more realistic estimate of the 1-sigma uncertainty in the ORIGEN-S fission product decay heat predictions is likely closer to about 4%.

[3] The lower bound of this range, that is, 6.4%, was calculated by adding contributions to error in quadrature, assuming absence of any correlation between the fission product and actinide components of decay heat. The upper bound, 9.0%, on the other hand, is calculated by adding the fission product and actinide error components linearly, that is, assuming that there is a strong correlation between the two constituents of decay heat.

6.5.4 Total Uncertainty in the Decay Heat Calculations

For a discharge burn-up of 260 MWh/kgU and decay time of 15 years, the uncertainty for ORIGEN-S predicted decay heat was estimated to range between 6.4% and 9.0%. To account for the uncertainty in the discharge burn-up, a 1% uncertainty is added yielding a range of 7.4% to 10% uncertainty in the decay heat calculations presented in this assessment.

7. CONCLUSIONS

The decay heat for 22 representative bundles out of 384 bundles in DSC-812 was calculated with ORIGEN-S using bundle data extracted from the NuFLASH fuel accounting database and the SORO production database. It is evident that the ORIGEN-S predicted decay heat for a representative bundle is independent of the bundle power history. Finally, the upper-bound 1-sigma uncertainty in the predicted decay heat calculations at decay times between 10 and 15 years is estimated to be 10%.

ACKNOWLEDGEMENTS

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Table 1: Bundle Data from NuFLASH and SORO

	NuFLASH				SORO			
Bundle Serial #	Channel Position Prior to Discharge	Discharge Date (yyyymmdd)	Uranium Mass (kg)	Module Position[4] (1 = Flare End, 2 = non-Flare End)	Channel Position Prior to Discharge	Discharge Date (yyyymmdd)	Fuel Type[5]	Discharge Burnup (MWh/kgU)
L90964C	k21-13	19930101	19.280	B0966-A06/1	k21-13	19930101	7	169.57
K23334Z	m02-13	19921220	19.340	B0962-D11/2	m02-13	19921220	7	198.82
K13749Z	q02-09	19921113	19.340	B0968-A06/1	q02-09	19921113	7	191.01
K37331Z	s20-11	19921216	19.340	B0962-G06/2	s20-11	19921216	7	173.20
K23722Z	x13-10	19930102	19.358	B0965-A06/1	x13-10	19930102	7	203.59
K23683Z	x13-11	19930102	19.331	B0965-A06/2	x13-11	19930102	7	216.69
K11377Z	e11-13	19921226	19.393	B0966-F05/2	e11-13	19921226	7	175.05
K36759Z	g20-12	19930101	19.331	B0965-C12/2	g20-12	19930101	7	188.61
K11339Z	h22-13	19921231	19.419	B0965-G10/1	h22-13	19921231	7	147.73
K36419Z	x07-06	19921219	19.393	B0962-C04/1	x07-06	19921219	7	150.45
K07950Z	x18-10	19921217	19.367	B0962-E02/1	x18-10	19921217	7	172.37
K08380Z	x18-11	19921217	19.411	B0962-E02/2	x18-11	19921217	7	183.42
K08307Z	x18-12	19921217	19.437	B0962-F01/1	x18-12	19921217	7	171.78
L77222C	b17-09	19921226	19.272	B0966-H11/2	b17-09	19921226	7	158.88
K27259Z	c07-13	19921217	19.367	B0962-H09/2	c07-13	19921217	7	157.27
K07258Z	j16-13	19930102	19.331	B0965-C06/1	j16-13	19930102	7	158.83
L90248C	o23-13	19921226	19.295	B0966-H01/2	o23-13	19921226	7	170.59
Q00877C	p08-11	19921226	19.354	B0966-G06/2	p08-11	19921226	7	205.64
L94448C	q14-10	19921228	19.298	B0966-C08/1	q14-10	19921228	7	159.96
L82133C	q16-10	19930104	19.241	B0968-C02/1	q16-10	19930104	7	227.71
L90687C	s13-13	19921226	19.278	B0966-H03/2	s13-13	19921226	7	162.00
K26434Z	t11-10	19930104	19.120	B0968-C04/1	t11-10	19930104	7	182.38

[4] Although NuFLASH contains accurate rack positions at BNGS-B, fuel handling staff does not have procedures in place to prevent the rotation of racks and trays prior to module loading. Since each tray is loaded into two rows within a module, bundle position accuracy may be limited to knowing that the bundle is in one of two rows (e.g. if bundle is slot H11 (flare end), it may actually be anywhere in rows G or H (12 bundle positions total).

[5] SORO Fuel Type 7 at Bruce NGS B is 37-element natural uranium.

Table 2: Decay Power at 2007-09-30 and 10 Years after Discharge

Bundle ID	Module Position[6]	NuFLASH U Mass (kg)	NuFLASH Burnup (MWh/kgU)	ORIGEN-S Burnup (MWh/kgU)	Discharge (Date)	Cooling Time at 09/30/07 (days)	Thermal Power at 2007-9-30 (W)	Thermal Power at 10 Years Cooling Time (W)
L90964C	B0966-A06/1	19.280	169.57	169.14	01/01/93	5385	3.608	4.073
K23334Z	B0962-D11/2	19.340	198.82	199.6	12/20/92	5397	4.221	4.772
K13749Z	B0968-A06/1	19.340	191.01	188.99	11/13/92	5434	4.020	4.568
K37331Z	B0962-G06/2	19.340	173.20	171.69	12/16/92	5401	3.681	4.173
K23722Z	B0965-A06/1	19.358	203.59	204.16	01/02/93	5384	4.327	4.902
K23683Z	B0965-A06/2	19.331	216.69	216.46	01/02/93	5384	4.559	5.161
K11377Z	B0966-F05/2	19.393	175.05	175.22	12/26/92	5391	3.753	4.240
K36759Z	B0965-C12/2	19.331	188.61	186.43	01/01/93	5385	3.976	4.500
K11339Z	B0965-G10/1	19.419	147.73	147.72	12/31/92	5386	3.191	3.600
K36419Z	B0962-C04/1	19.393	150.45	149.68	12/19/92	5398	3.235	3.662
K07950Z	B0962-E02/1	19.367	172.37	171.53	12/17/92	5400	3.662	4.143
K08380Z	B0962-E02/2	19.411	183.42	183.80	12/17/92	5400	3.913	4.420
K08307Z	B0962-F01/1	19.437	171.78	170.81	12/17/92	5400	3.642	4.104
L77222C	B0966-H11/2	19.272	158.88	159.13	12/26/92	5391	3.410	3.860
K27259Z	B0962-H09/2	19.367	157.27	161.30	12/17/92	5400	3.456	3.904
K07258Z	B0965-C06/1	19.331	158.83	159.61	01/02/93	5384	3.426	3.870
L90248C	B0966-H01/2	19.295	170.59	171.06	12/26/92	5391	3.641	4.110
Q00877C	B0966-G06/2	19.354	205.64	205.70	12/26/92	5391	4.372	4.964
L94448C	B0966-C08/1	19.298	159.96	159.23	12/28/92	5389	3.429	3.885
L82133C	B0968-C02/1	19.241	227.71	230.93	01/04/93	5382	4.852	5.516
L90687C	B0966-H03/2	19.278	162.00	163.01	12/26/92	5391	3.483	3.936
K26434Z	B0968-C04/1	19.120	182.38	186.32	01/04/93	5382	3.941	4.468

[6] Although NuFLASH contains accurate rack positions at BNGS-B, fuel handling staff does not have procedures in place to prevent the rotation of racks and trays prior to module loading. Since each tray is loaded into two rows within a module, bundle position accuracy may be limited to knowing that the bundle is in one of two rows (e.g. if bundle is slot H11 (flare end), it may actually be anywhere in rows G or H (12 bundle positions total).

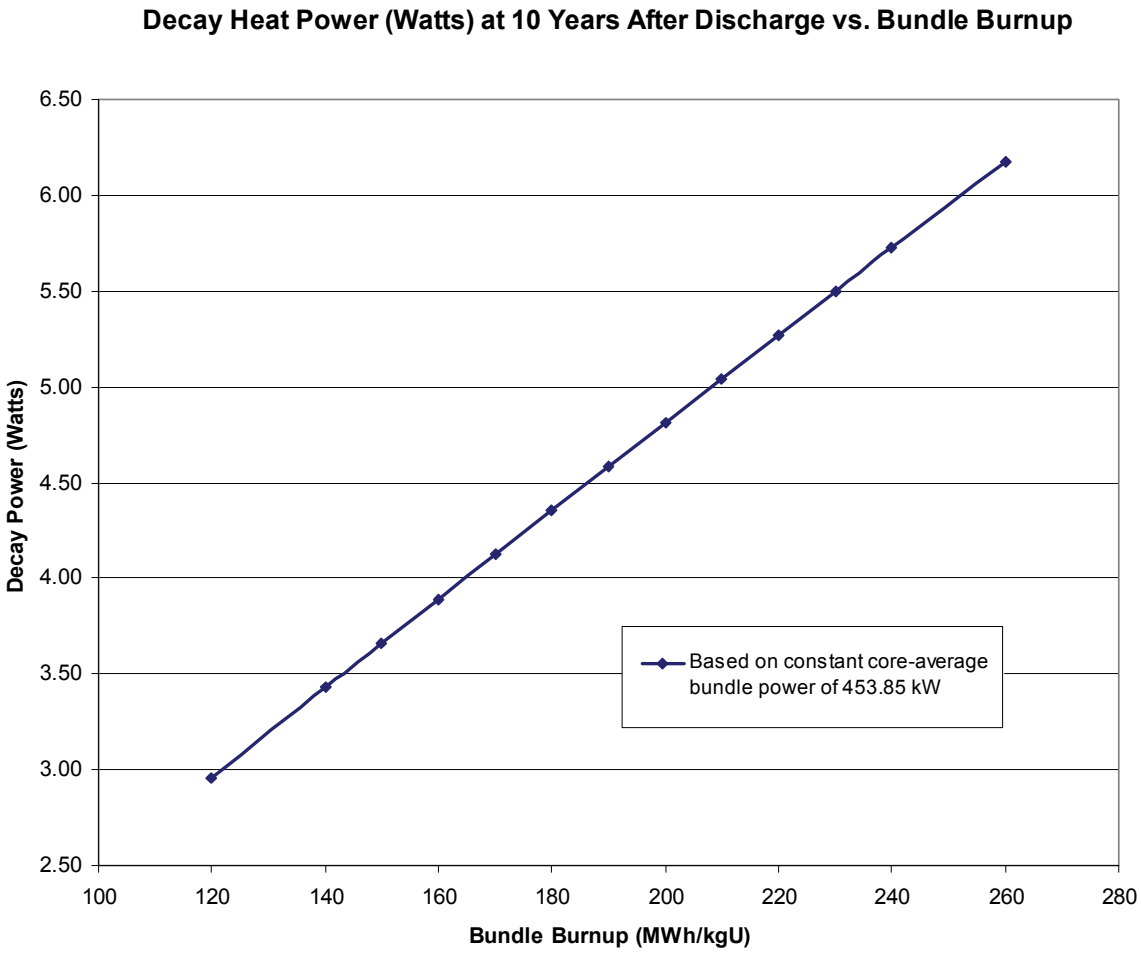

Figure 1: Reference Curve

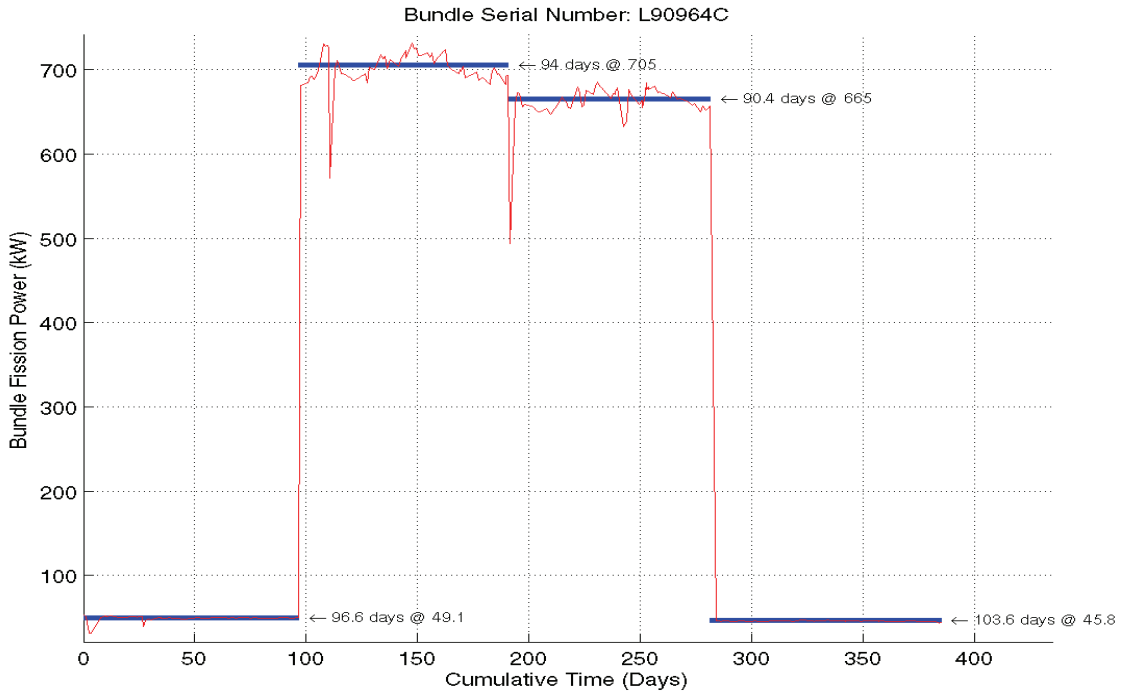

Figure 2: Block Average Bundle Power History for L09064C

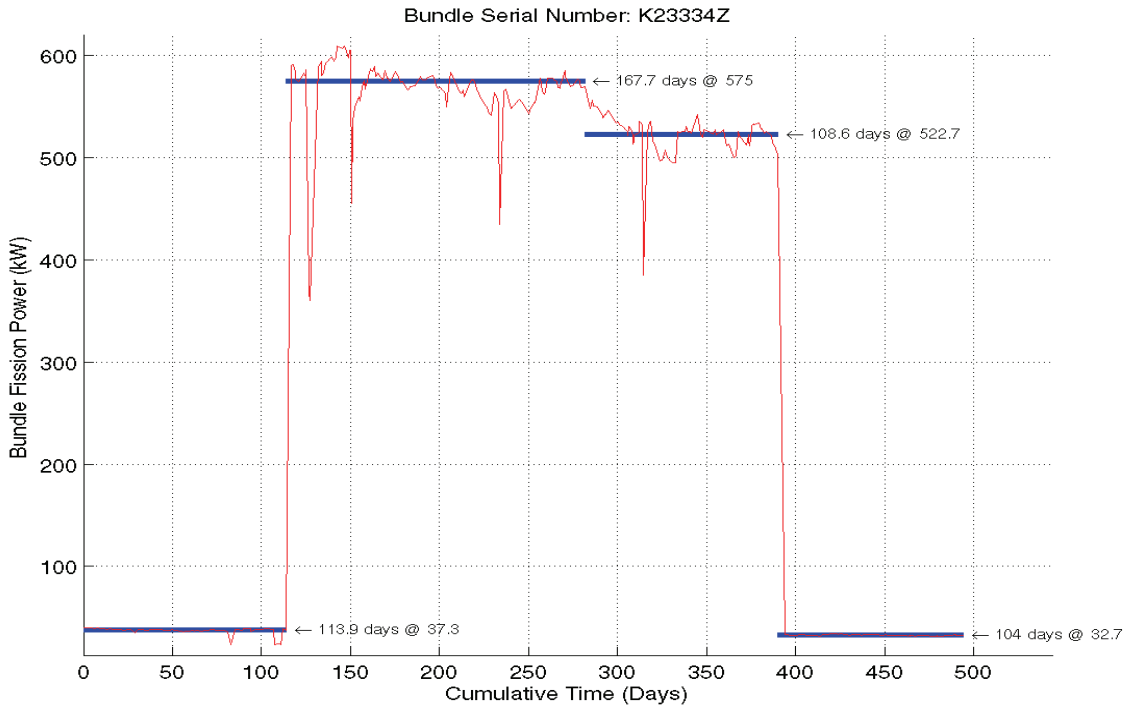

Figure 3: Block Average Bundle Power History for K23334Z

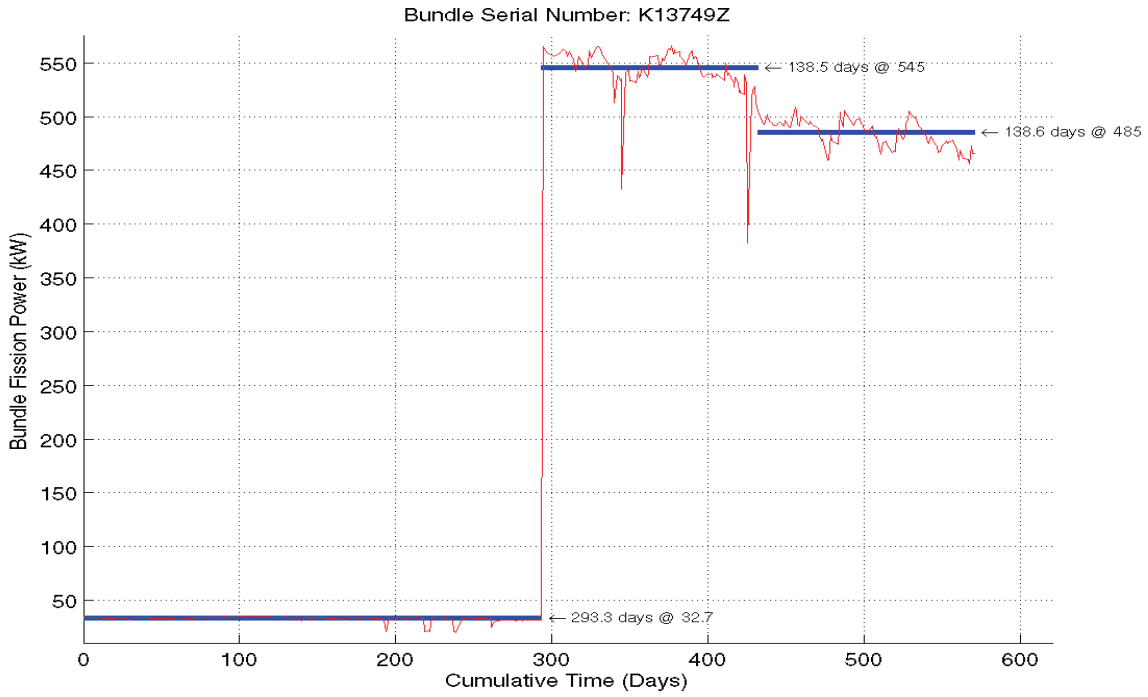

Figure 4: Block Average Bundle Power History for K13749Z

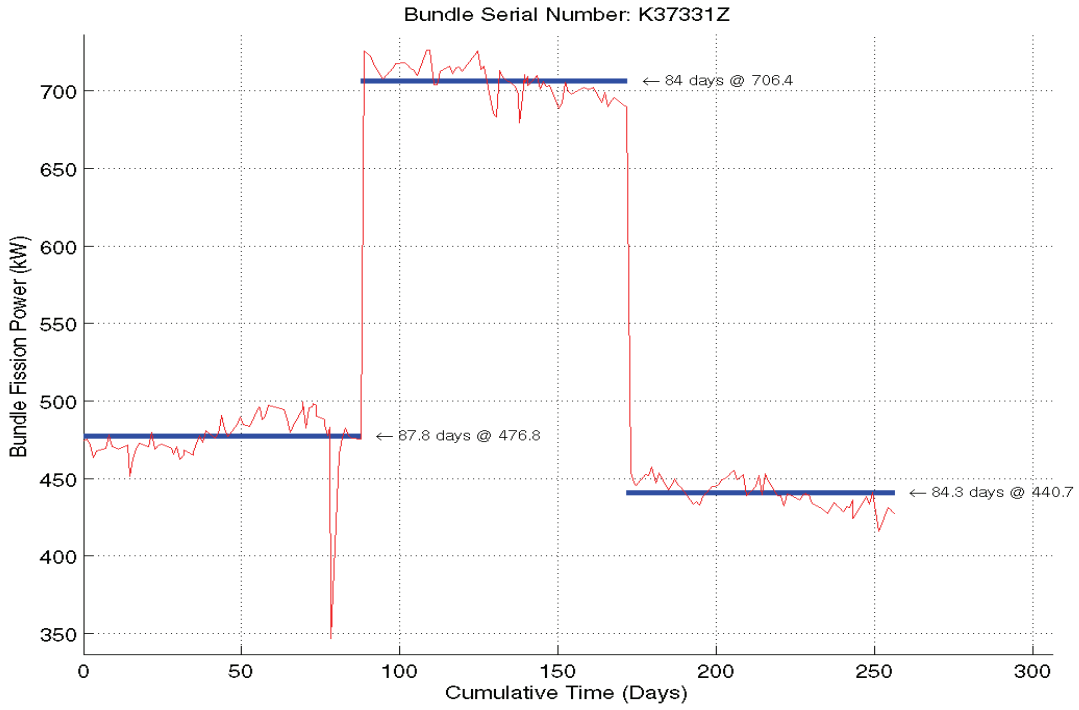

Figure 5: Block Average Bundle Power History for K37331Z

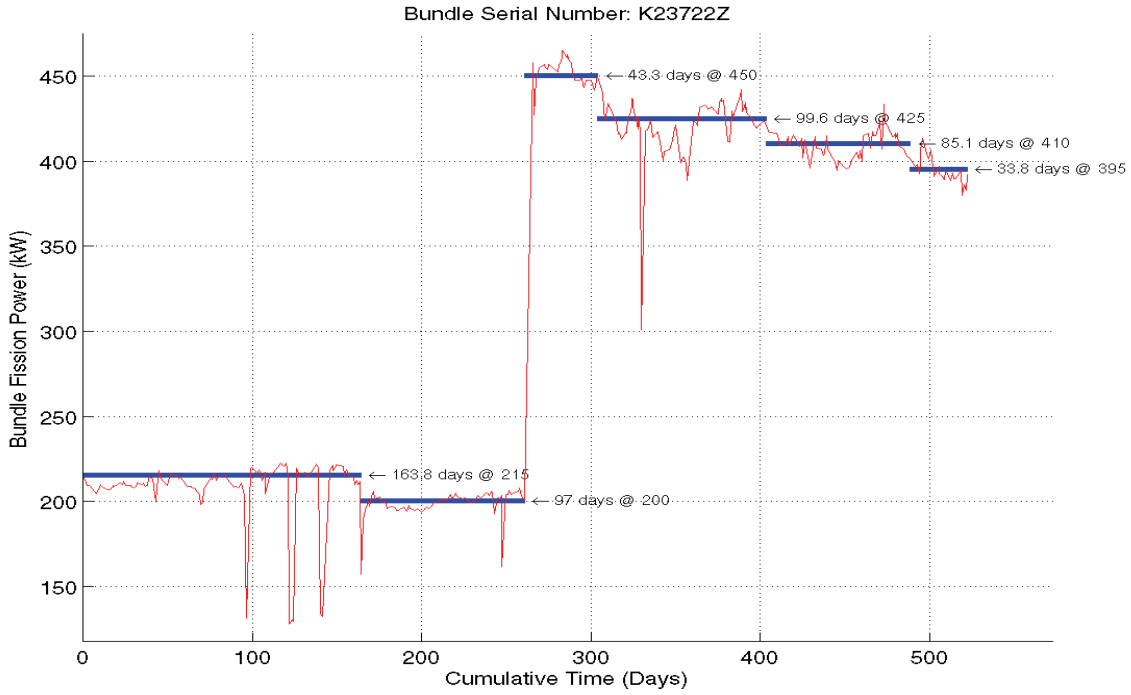

Figure 6: Block Average Bundle Power History for K23722Z

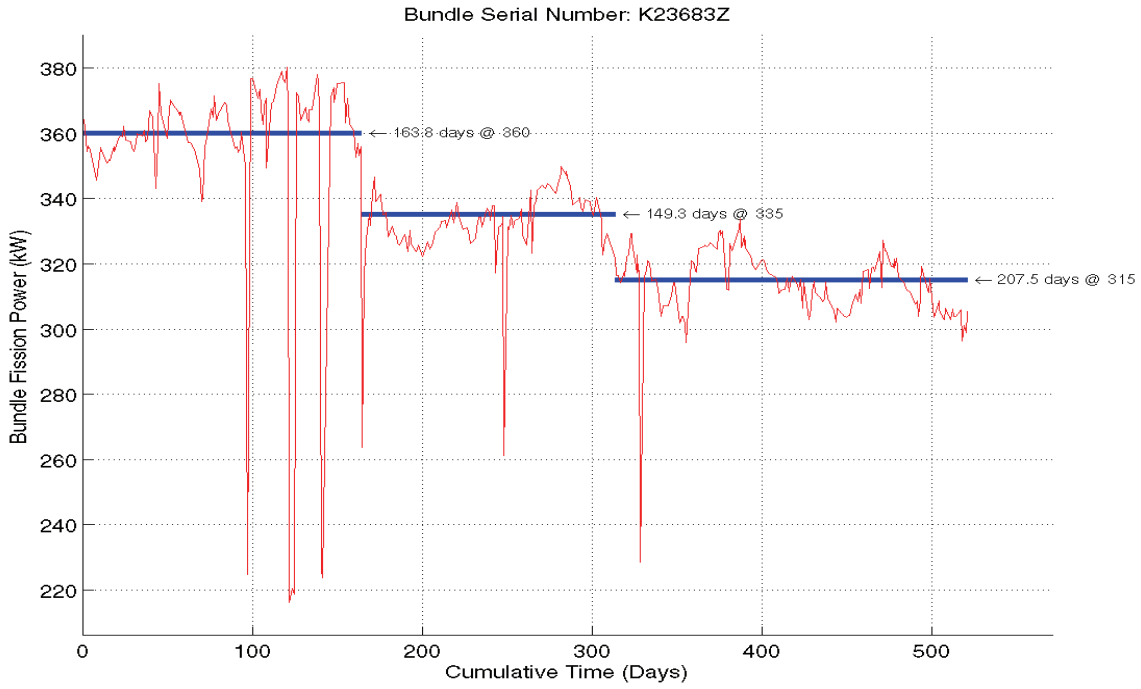

Figure 7: Block Average Bundle Power History for K23683Z

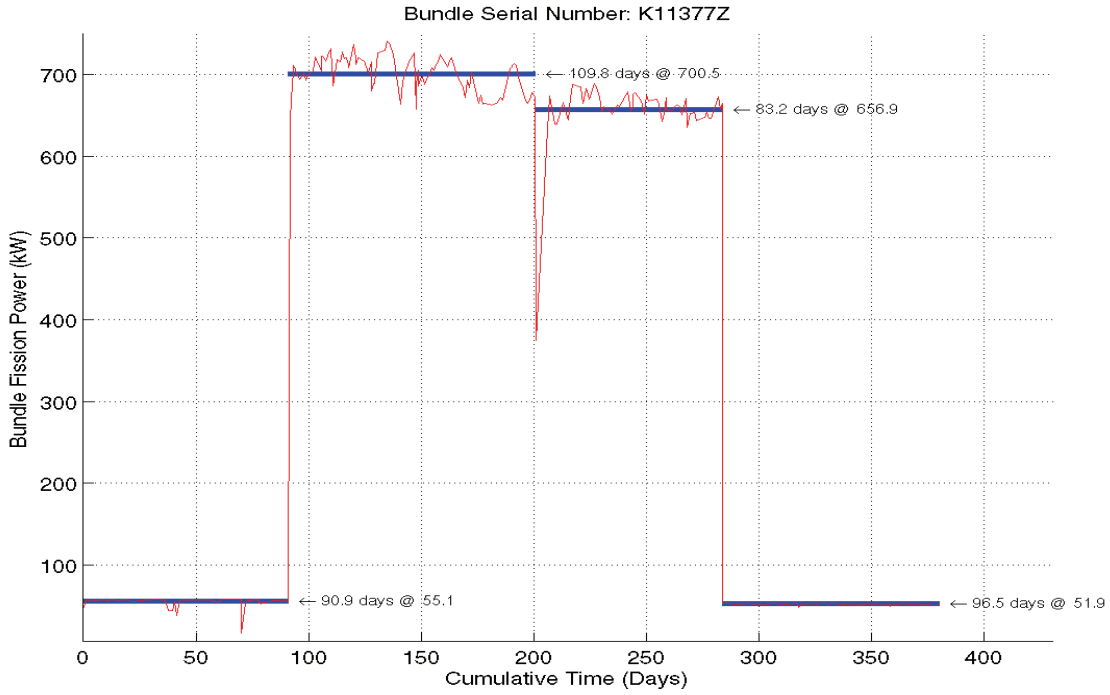

Figure 8: Block Average Bundle Power History for K11377Z

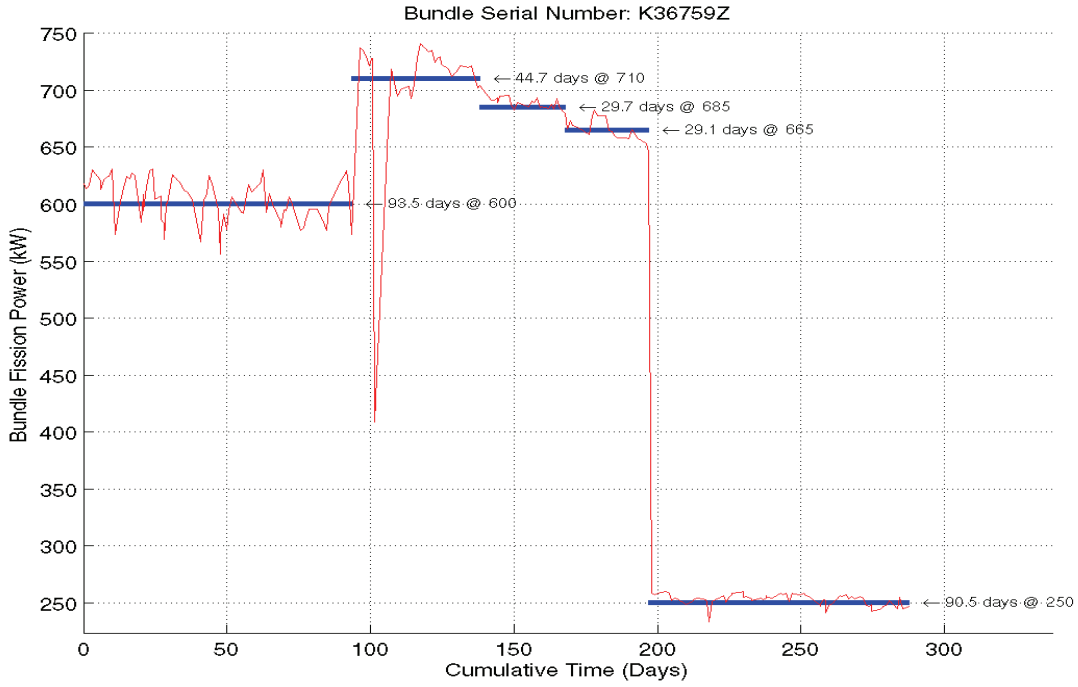

Figure 9: Block Average Bundle Power History for K36759Z

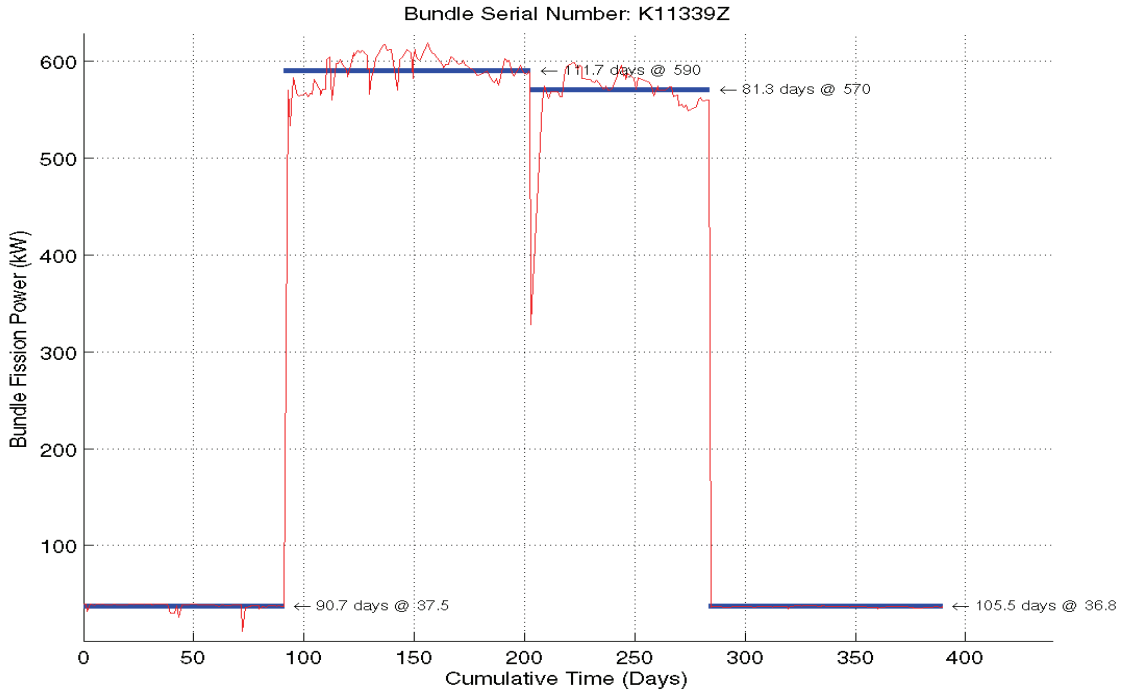

Figure 10: Block Average Bundle Power History for K11339Z

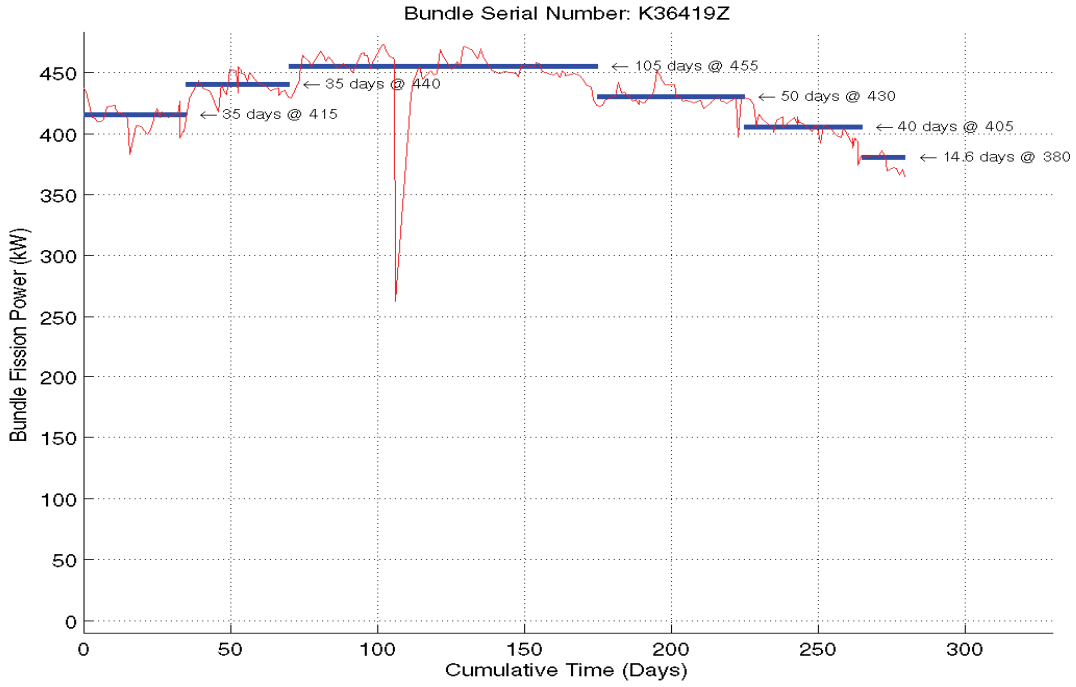

Figure 11: Block Average Bundle Power History for K36419Z

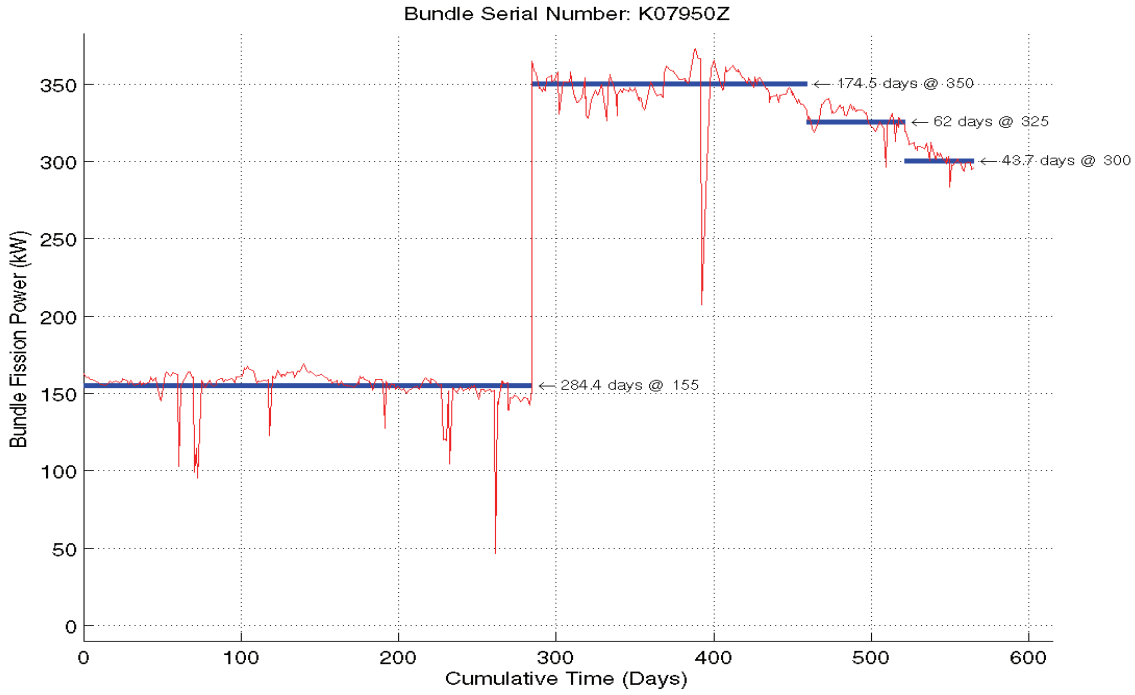

Figure 12: Block Average Bundle Power History for K07950Z

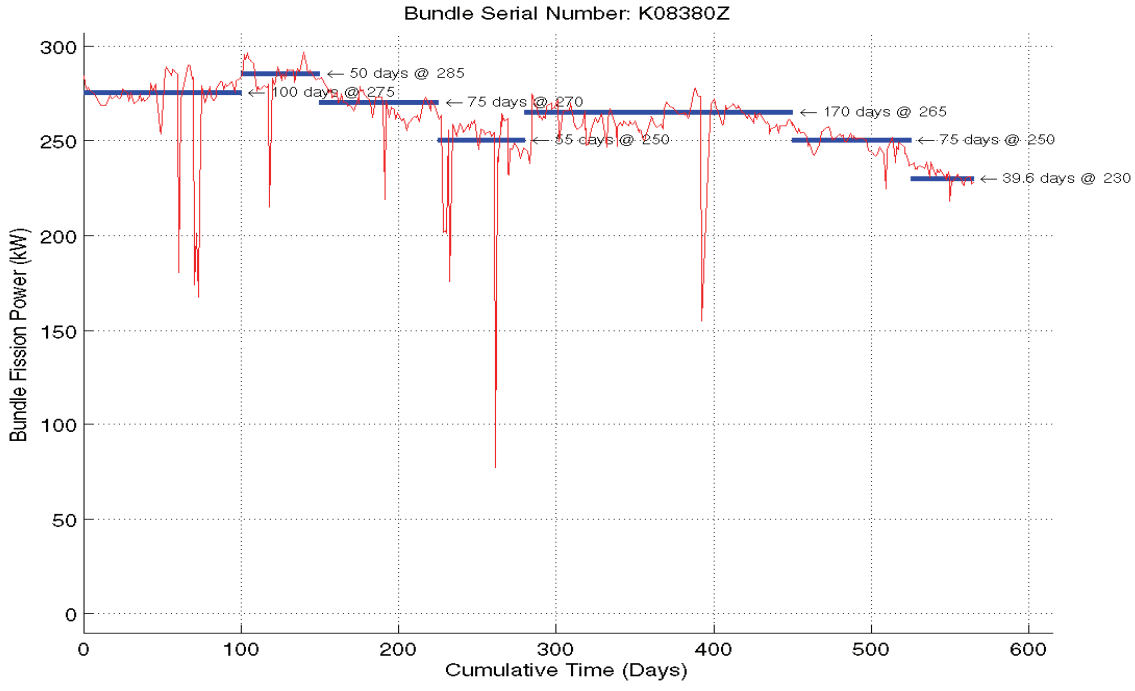

Figure 13: Block Average Bundle Power History for K08380Z

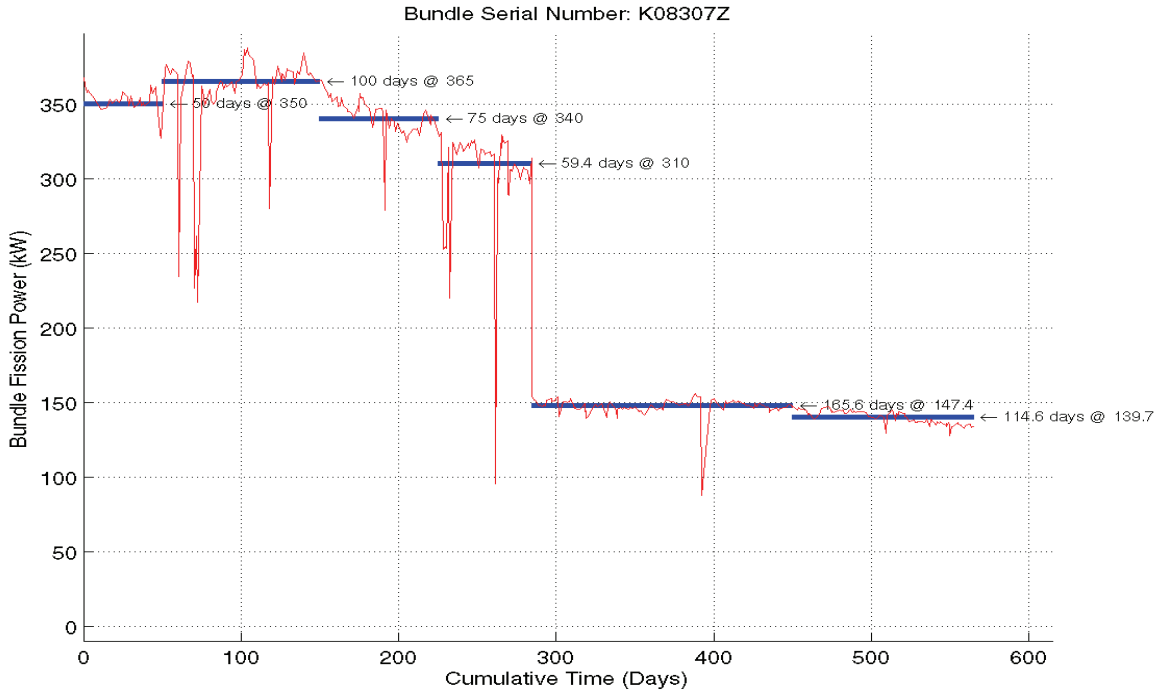

Figure 14: Block Average Bundle Power History for K08307Z

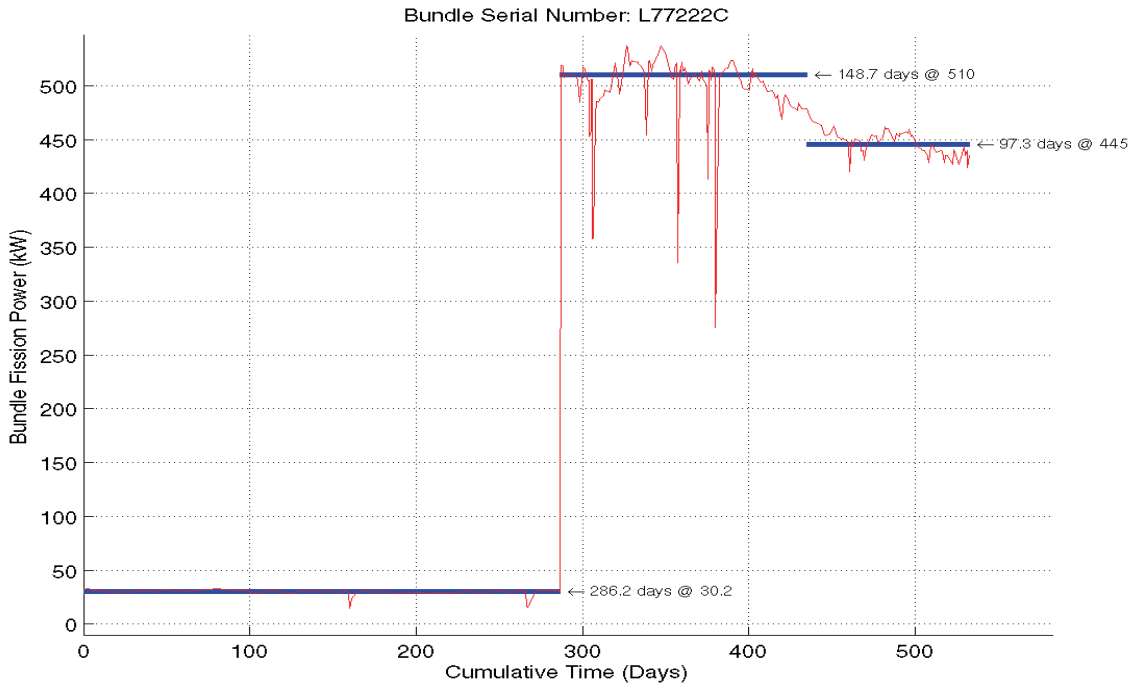

Figure 15: Block Average Bundle Power History for L77222C

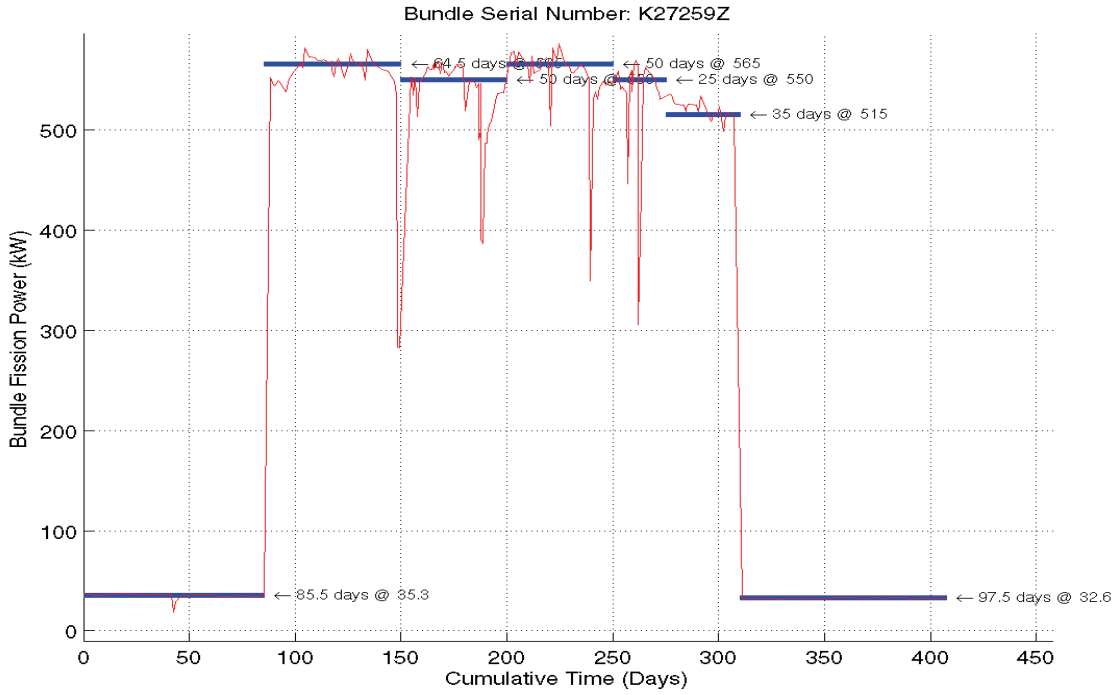

Figure 16: Block Average Bundle Power History for K27259Z

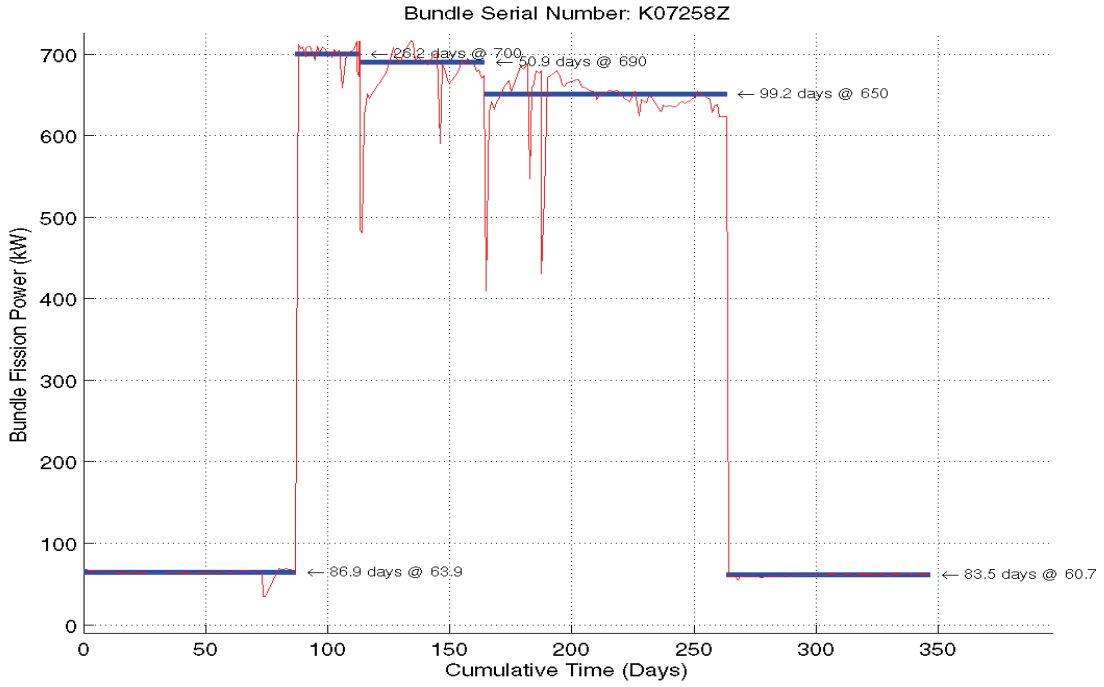

Figure 17: Block Average Bundle Power History for K07258Z

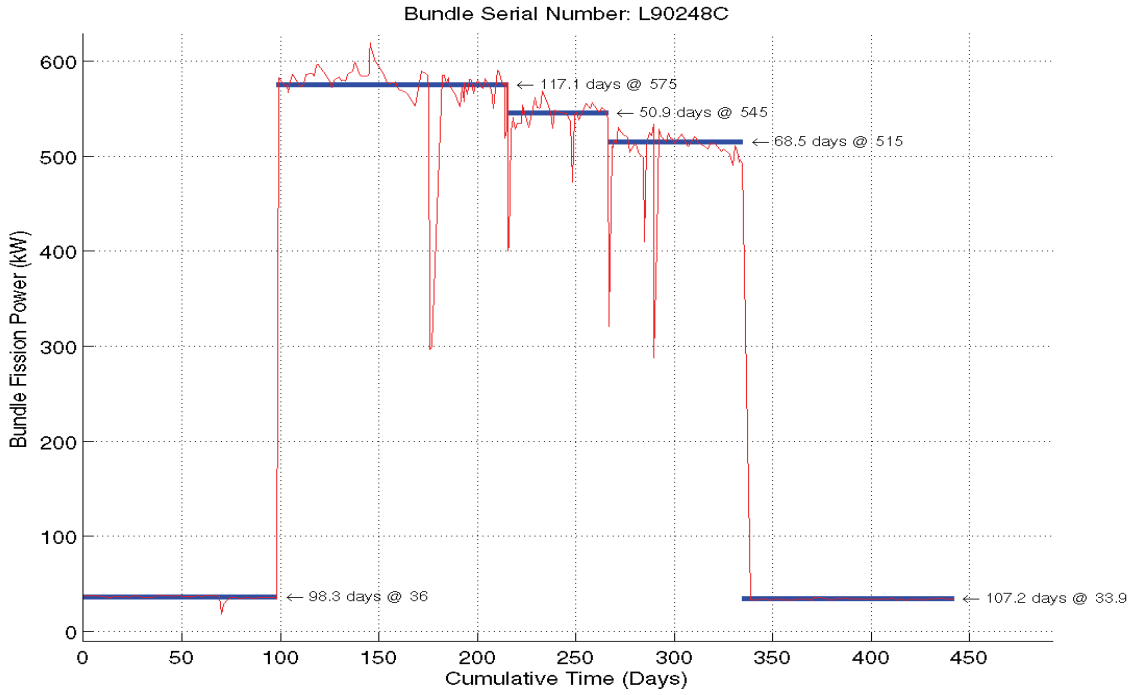

Figure 18: Block Average Bundle Power History for L90248C

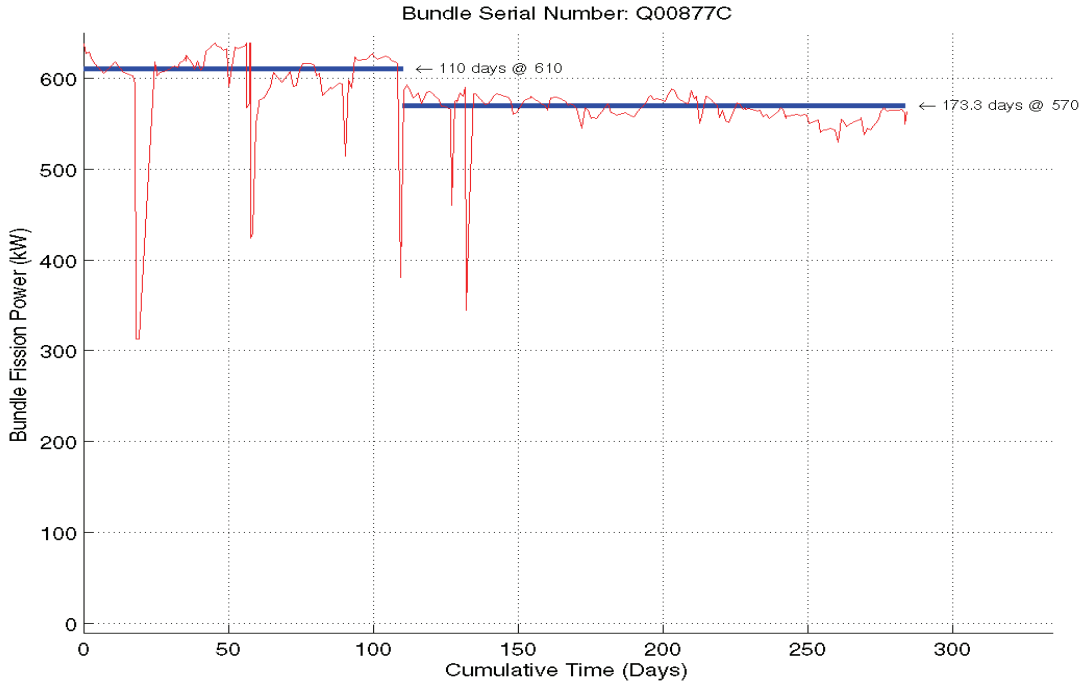

Figure 19: Block Average Bundle Power History for Q00877C

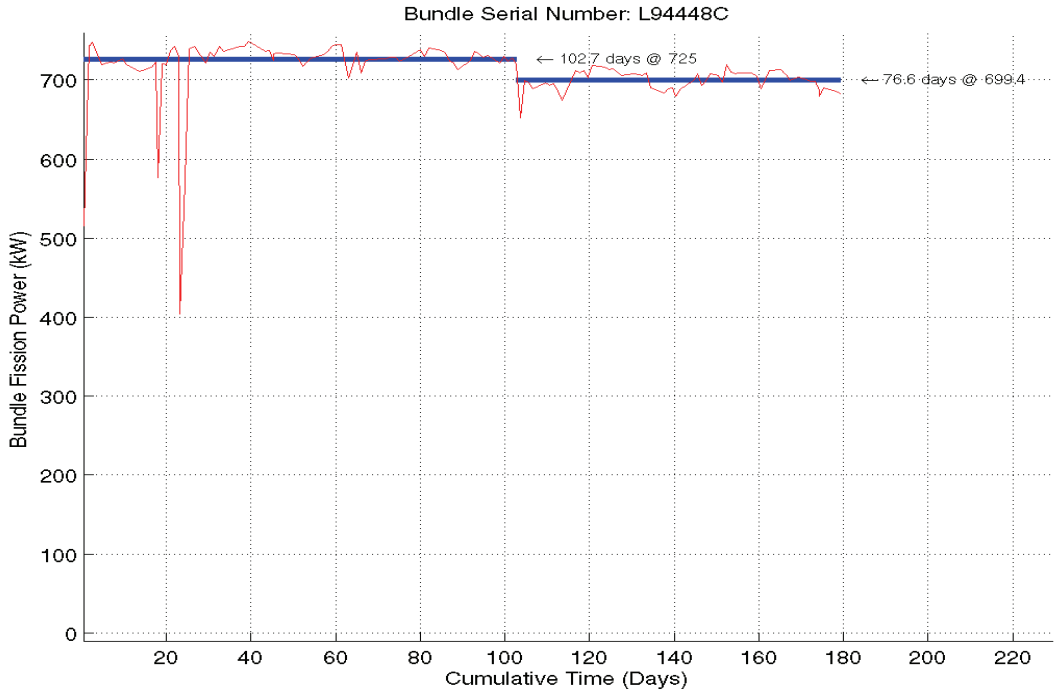

Figure 20: Block Average Bundle Power History for L94448C

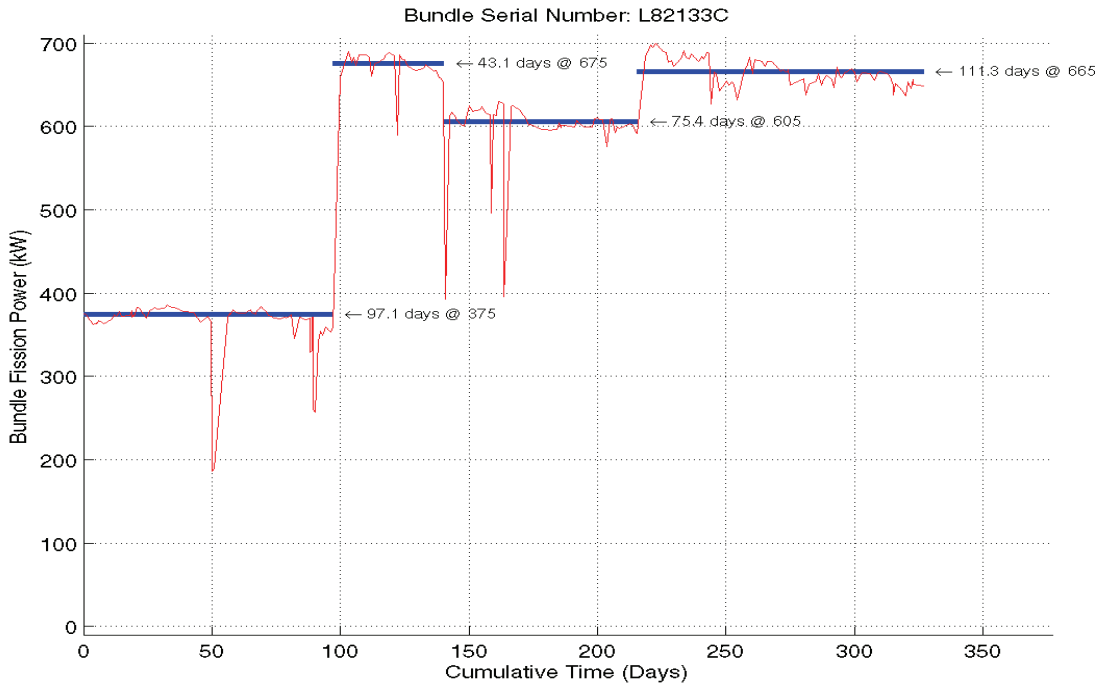

Figure 21: Block Average Bundle Power History for L82133C

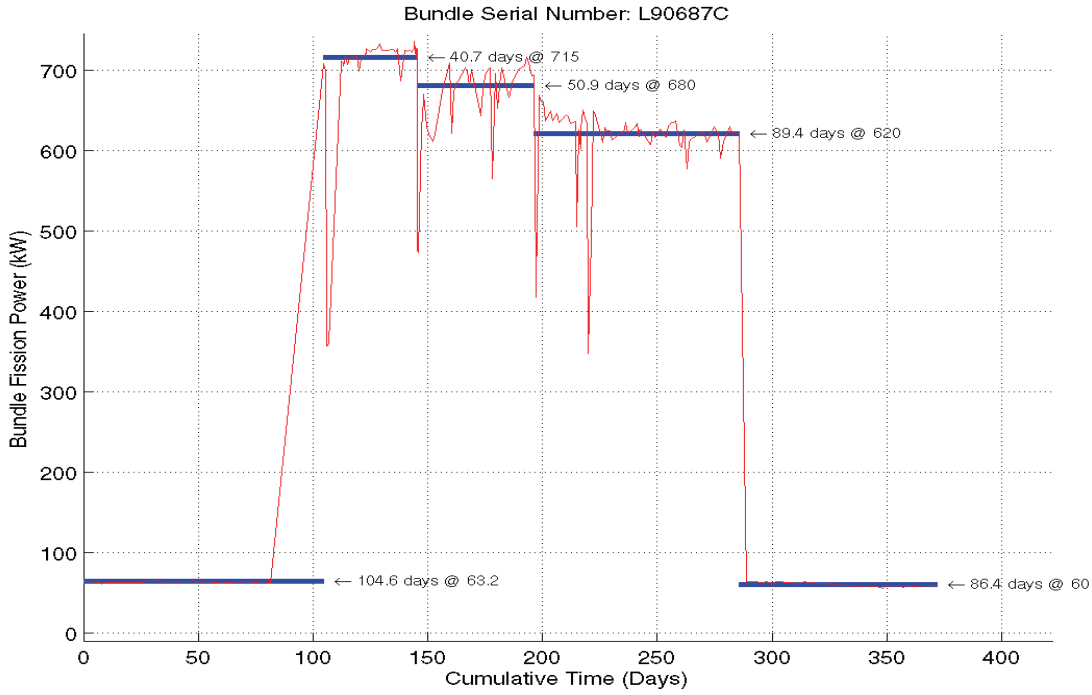

Figure 22: Block Average Bundle Power History for L90687C

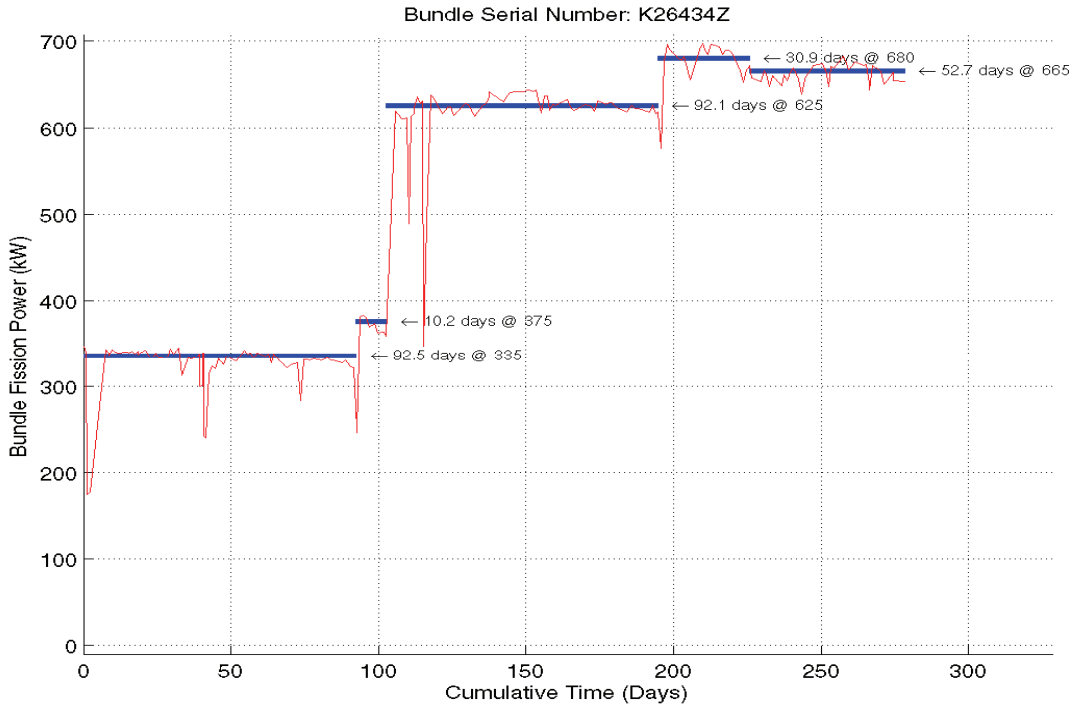

Figure 23: Block Average Bundle Power History for K26434Z

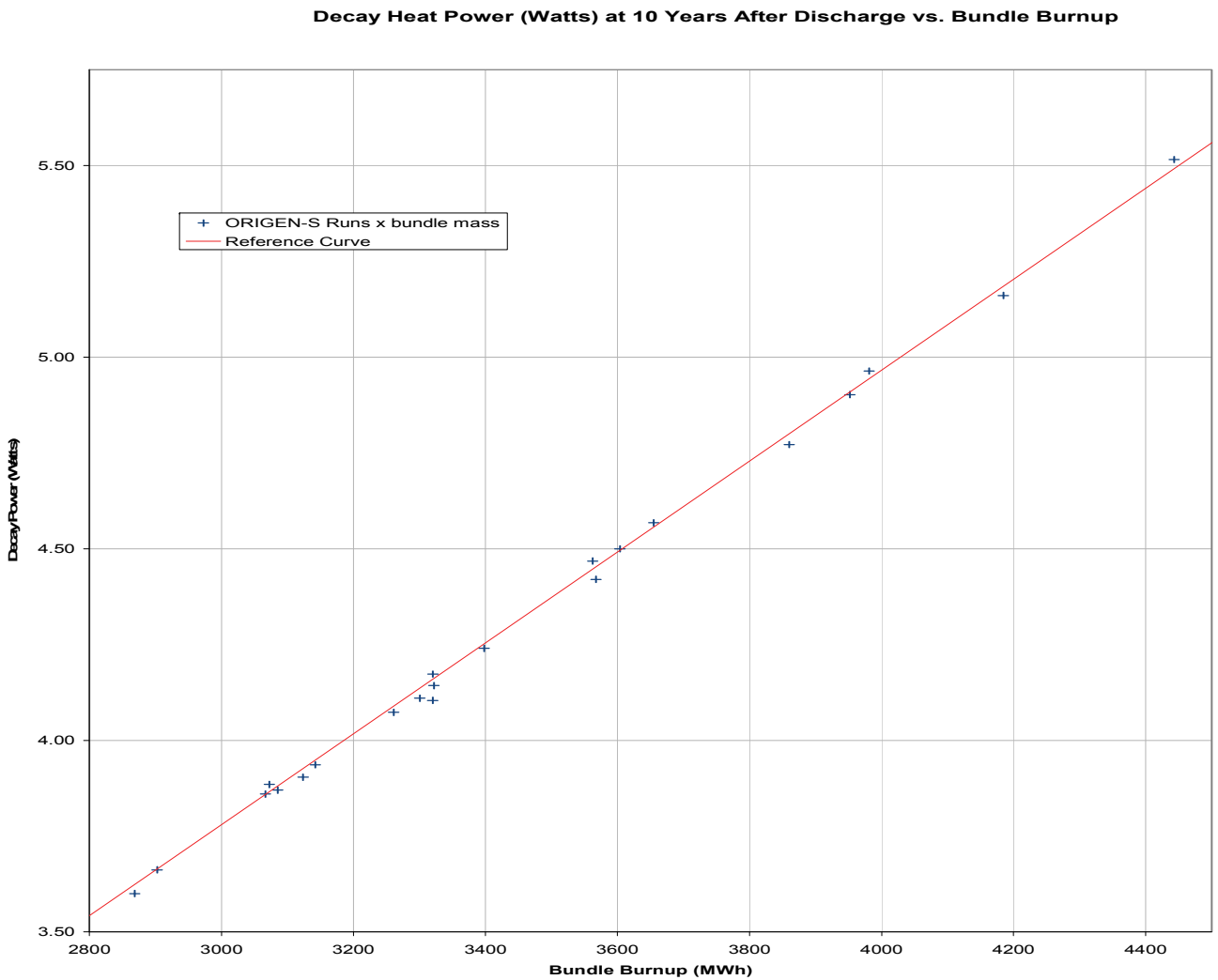

Figure 24: ORIGEN-S Calculated Decay Heat at 10 Years Compared with Reference Curve