Thermal Properties for the Thermal-Hydraulics Analyses of the BR2 Maximum Nominal Heat Flux

Rev. 1

Nuclear Engineering Division

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February 2015

prepared for

U. S. Department of Energy, National Nuclear Safety Administration, Office of Global Threat
Reduction (NA-21)

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1. Introduction

This memo describes the assumptions and references used in determining the thermal properties for the various materials used in the BR2 HEU (93% enriched in ^{235}U) to LEU (19.75% enriched in ^{235}U) conversion feasibility analysis. More specifically, this memo focuses on the materials contained within the pressure vessel (PV), i.e., the materials that are most relevant to the study of impact of the change of fuel from HEU to LEU.

Section 2 provides a summary of the thermal properties in the form of tables while the following sections and appendices present the justification of these values. Section 3 presents a brief background on the approach used to evaluate the thermal properties of the dispersion fuel meat and specific heat capacity. Sections 4 to 7 discuss the material properties for the following materials: i) aluminum, ii) dispersion fuel meat ($\text{UAl}_x\text{-Al}$ and U-7Mo-Al), iii) beryllium, and iv) stainless steel. Section 8 discusses the impact of irradiation on material properties. Section 9 summarizes the material properties for typical operating temperatures. Appendix A elaborates on how to calculate dispersed phase's volume fraction. Appendix B provides a revised methodology for determining the thermal conductivity as a function of burnup for HEU and LEU.

2. Thermal properties summary tables

Table 1 shows the proposed conservative temperature-independent values of the thermal properties for use in BR2 analyses, as described in this document.

Table 1 Conservative temperature-independent value for the thermal properties.

	Thermal conductivity (k_t) W/m-K	Specific heat capacity (C_p) J/kg-K	Density (ρ) kg/m ³	ρC_p (J/m ³ -K)
AG3NE cladding	130	880	2670	2349600
Al 6061-T6	167	896	2700	2419200
Beryllium (unirradiated)	149	1925	1836	3534300
Beryllium (long irradiation)	50	-	-	-
Stainless steel 304	16	500	8000	4000000
$\text{UAl}_x\text{-Al}$ dispersion (fresh)	80	646	3580	2312366
U-7Mo-Al dispersion (fresh)	66	275	9870	2714250
$\text{UAl}_x\text{-Al}$ dispersion ($\beta^*=25\%$)	69	-	-	-
U-7Mo-Al dispersion ($\beta=25\%$)	41	-	-	-

* β = %at of ^{235}U depleted (burnup)

Table 2 gives the tabulated values of the volumetric heat capacity as a function of temperature for the BR2 HEU fresh fuel meat ($\text{UAl}_x\text{-Al}$).

Table 2 Tabulated volumetric heat capacity for BR2 fresh HEU fuel meat (UAl_x-Al).

Temperature		ρC_p (J/m ³ -K)
°C	K	
20	293.15	2312366
50	323.15	2319057
100	373.15	2330207
150	423.15	2341357
200	473.15	2352507

Table 3 gives the tabulated values of the thermal conductivity as a function of temperature for the BR2 LEU fresh fuel meat (U-7Mo-Al).

Table 3 Tabulated thermal conductivity for BR2 fresh LEU fuel meat (U-7Mo-Al).

Temperature		k_t (W/m-K)
°C	K	
20	293.15	65.6
50	323.15	66.9
100	373.15	69.0
150	423.15	71.1
200	473.15	73.0

Table 4 gives the tabulated values of the thermal conductivity as a function of temperature for beryllium.

Table 4 Tabulated thermal conductivity for fresh beryllium.

Temperature		k_t (W/m-K)
°C	K	
20	293.15	190
50	323.15	183
100	373.15	172
150	423.15	161
200	473.15	149

The above tables provide a summary of the materials properties as justified in this document. However, a revised method for determining the thermal conductivity of the UAl_x-Al and U-7Mo-Al dispersion fuel as a function of burnup has been developed and is described in Appendix B. A summary of these thermal conductivity values is given in Table 5.

Table 5 Thermal conductivity of dispersion fuel as function of burnup, as described in Appendix B.

	Thermal conductivity (k_t) W/m-K
UAl _x -Al dispersion ($\beta=0$)	80.5
UAl _x -Al dispersion ($\beta=16\%$)	64.1
UAl _x -Al dispersion ($\beta=32\%$)	51.2
UAl _x -Al dispersion ($\beta=46\%$)	43.9
U-7Mo-Al dispersion ($\beta=0\%$)	86.1
U-7Mo-Al dispersion ($\beta=16\%$)	36
U-7Mo-Al dispersion ($\beta=32\%$)	23.5
U-7Mo-Al dispersion ($\beta=46\%$)	19.4

* β = % at of ²³⁵U depleted (burnup)

3. Approach for the evaluation of fuel meat thermal properties

This section presents a brief background on the approach used to evaluate the thermal properties of the thermal conductivity and specific heat capacity of the current HEU and the proposed LEU dispersion fuel meats.

3.1 Dispersion fuel meat thermal conductivity

Thermal properties of the dispersion fuel meat need to be evaluated for the specific uranium loading in the BR2 HEU (UAl_x-Al) and proposed LEU (U-7Mo-Al) fuel meats.

To obtain the thermal conductivity of the dispersion fuel meat, Ref. [1] proposes the use of the following formula:

$$k_{meat} = \frac{-f + 3Vf + 2m - 3Vm + \sqrt{8fm + (f - 3Vf - 2m + 3Vm)^2}}{4}, \quad (1)$$

where k_{meat} is the effective thermal conductivity of the fuel meat, f is the composite thermal conductivity of the fuel and reaction-product phase, m is the thermal conductivity of the aluminum matrix phase, and V is the sum of the volume fractions of the fuel and reaction-product phases.

For the BR2 feasibility analysis, the thermal conductivity of the reaction-product phase will be assumed to be the same as the fuel particle. Note that the thermal conductivity associated with the fuel particle, aluminum matrix and reaction-product phase need to be corrected for porosity (either from fabrication or irradiation) using the following formula [3]

$$k_p = k_{100} \cdot \exp(-2.14P) \quad (2)$$

where P is the porosity fraction, and k_{100} is the thermal conductivity without porosity.

3.2 Specific heat capacity

When reference data is unavailable for a given material, the specific heat capacity is obtained through the mixture rule shown in Eq. (3),

$$C_{p,mixture} = \sum_i f_i \times C_{p,i} , \quad (3)$$

where i is the index of each component, f_i is the mass fraction of each component, and $C_{p,i}$ is the specific heat capacity of each component given in J/kg-K..

Since none of the analyses planned for BR2 will model changes in solid materials volumes due to thermal expansion, the nominal density is kept constant in order to preserve the mass of a given material. Therefore, the change in volumetric heat capacity (ρC_p) with temperature is represented only by the variation of specific heat capacity with temperature.

4. Cladding and structure thermal properties (aluminum)

4.1 Thermal conductivity

For the aluminum matrix of both fuels (pure aluminum), a thermal conductivity of 210 W/m-K is reported in Ref. [2]. Ref. [19] reports a thermal conductivity closer to 240 W/m-K near room temperature which decreases near around 210 W/m-K near the melting point. It is proposed that the fuel meat thermal properties be calculated using 210 W/m-K as a temperature independent thermal conductivity for aluminum matrix.

Historically, BR2 has assumed a thermal conductivity of 150 W/m-K [4] for its cladding (AG3NE or AISI5754 alloy). The 5000 aluminum alloy series (see Ref. [9]) have thermal conductivities varying between 108 and 205 W/m-K [5] with an average of 143 W/m-K. Ref. [6] states that thermal conductivity of the AG3NE is about 130 W/m-K. It is proposed that 130 W/m-K is used as a temperature-independent thermal conductivity for the BR2 fuel cladding.

A thermal conductivity of 167 W/m-K is reported in Ref. [11] for the aluminum alloy 6061-T6 (assumed for Al structures inside the PV). Ref. [19] reports the typical value of 180 W/m-K. It is proposed that 167 W/m-K is used as a temperature-independent thermal conductivity for the BR2 aluminum structures inside the PV.

4.2 Specific heat capacity

For the aluminum matrix of both fuels (pure aluminum), a specific heat capacity of 0.900 J/g-K is reported in Ref. [2]. Ref. [20] reports specific heat capacity ranging from 0.9000 at 300K to 1.2224 at 900K. It proposed that 0.900 J/g-K is used as a temperature-independent specific heat capacity.

For the cladding, the specific heat capacities of the 5000 aluminum series vary between 0.880 J/g-K and 0.904 J/g-K with an average of 0.897 J/g-K [5]. Ref. [6] states the specific heat capacity of AG3NE is 0.96 J/g-K. Using Eq. 3 and the weight fractions of the alloy constituents [14, [15], a heat capacity of 0.901 J/g-K is calculated. It proposed that 0.880 J/g-K is used as a temperature-independent specific heat capacity.

It is proposed that 0.896 J/g-K [11] be used for a temperature-independent specific heat capacity for aluminum 6061-T6.

4.3 Density

The density of pure aluminum is reported as 2.6989 g/cm³ [2]. For AG3NE (aluminum alloy 5754), the density is reported as 2.67 g/cm³ [15]. For the aluminum alloy 6061, the density is reported as 2.7 g/cm³ [11].

5. Fresh HEU fuel meat thermal properties (UAl_x-Al)

The current HEU fuel (UAl_x) is composed mainly of UAl₃ and UAl₄ dispersed in aluminum with a ratio of typically 60% and 40%, respectively [6]. The typical loading in a HEU BR2 fuel assembly (400g of ²³⁵U) requires a fuel meat density of 1.3 gU/cm³. To obtain such density, it is necessary to have 35.4 w/o (w_{heu fuel}) of fuel particles in the meat. This corresponds to a volume fraction of the dispersed phase in the meat of 29% (see appendix A). The typical porosity for those loadings has historically been assumed, in the RERTR program, to be 7% [6].

5.1 Thermal conductivity

The data related to thermal conductivity of UAl_x-Al in Ref. [6] is somewhat sparse.

The thermal conductivity of UAl alloy (in W/cm-K) can be represented by,

$$k_t = 2.17 - 2.76 w, \quad (4)$$

where w is the weight fraction of U in the alloy [6].

Then, assuming a value of 0.70 for w (calculated for an equivalent fuel particle made of 60% UAl₃ and 40% UAl₄), using Eqs 1 and 4, and the other assumptions at the beginning of Section 4, a thermal conductivity of 113 W/m-K is calculated for fresh UAl_x-Al fuel meat.

Another value for the UAl_x-Al fuel meat thermal conductivity can be extrapolated from Figure 1. The BR2 historical thermal conductivity of 80 W/m-K [4] can be obtained from this figure assuming about a 32% volume fraction of the combined fuel and porosity.

It is proposed that 80 W/m-K is used as a temperature-independent thermal conductivity for the UAl_x-Al fresh fuel meat.

The revised method for calculating the thermal conductivity of fresh HEU fuel meat is given in Appendix B.

Figure 1. Thermal conductivity vs volume percent of fuel and porosity [6].

5.2 Specific heat capacity

According to Ref. [6], the specific heat capacity (in J/g K) of the UAl_3 and UAl_4 fuel particles can be obtained by,

$$C_{p,UAl3} = 0.329 + 0.00021 T, \quad (5)$$

$$C_{p,UAl4} = 0.473 + 0.00024 T, \quad (6)$$

where T is the temperature in °C.

Using Eqs 3, 5 and 6, the specific heat capacity for the UAl_x fuel meat can be calculated using

$$C_{p,UAlx} = w_{matrix} C_{p,matrix} + w_{fuel} (0.6 C_{p,UAl3} + 0.4 C_{p,UAl4}) \quad (7)$$

where $w_{matrix} = (1 - w_{fuel})$.

Using Eq. 7, the tabulated specific heat capacity as a function of temperature is calculated and given in Table 2.

5.3 Density

The UAl_x -Al fuel meat density is calculated to be 3.58 g/cm^3 for the BR2 specific loading (see Appendix A).

6. Fresh LEU fuel meat thermal properties (U-7Mo-Al)

The proposed LEU fuel is composed of U-7Mo dispersed in aluminum at a density between 7.5 gU/cm^3 and 8.0 gU/cm^3 . Considering that the volume fraction of the dispersed phase is larger for higher loading (and results in a lower thermal conductivity and specific heat capacity), 8.0 gU/cm^3 is selected at this point to evaluate the thermal properties for conservative feasibility analysis.

To obtain 8.0 gU/cm^3 in the same geometry as HEU fuel assembly, it is necessary to have 80.9 w/o ($w_{\text{leu fuel}}$). This corresponds to a 49.07% volume fraction of the dispersed phase (see appendix A). Recent discussions with ANL fuel expert characterized the CERCA (fabricator of BR2 fuel) process as having an upper limit of about 4% porosity [7] for U-7Mo-Al fuel meat at BR2 proposed loading.

6.1 Thermal conductivity

According to Ref. 8, an estimate of k_t (in W/m-K) can be obtained for UMo alloy by

$$k_t = 2.2 + 0.032 T \quad (8)$$

where T is the temperature in K.

A slightly different relationship is presented in Ref. [17],

$$k_t = 0.034 T - 0.56 \quad (9)$$

where T is the temperature in K.

Eqs 1 and 8 (or 9) can be used to calculate the meat thermal conductivity as a function of temperature. At 20°C , the thermal conductivity predicted by Eqs. 1 and 8 is 68.4 W/m-K and 65.6 W/m-K using Eqs. 1 and 9. It is proposed that 66 W/m-K as a temperature-independent thermal conductivity for the U-7Mo-Al fresh fuel meat. Using Eq. 9, the tabulated thermal conductivity as a function of temperature is calculated and given in Table 3.

The revised method for calculating the thermal conductivity of fresh LEU fuel meat is given in Appendix B.

6.2 Specific heat capacity

The specific heat capacity (in J/mol-K) for the UMo fuel particles can be calculated using Eq. 10 [9].

$$C_{p,UMo} = 29.84 - 8.9E-3 T + 4.32E-5 T^2 - 2.06E-8 T^3 \quad (10)$$

Using Eq. 3, the aluminum matrix specific heat capacity, $w_{leu\ fuel}$, and a conversion factor (228.08 g/mol for U-7Mo), the specific heat capacity of the LEU fuel meat can be calculated. According to Eq. 10, the specific heat capacity varies between 0.2748 J/g-K and 0.2759 J/g-K in the range between 20 °C and 200 °C.

It is proposed that 0.275 J/g-K is used for a temperature-independent specific heat capacity for fresh LEU fuel (U-7Mo-Al).

6.2.1 6.3. Density

The U-7Mo-Al fuel meat density is calculated to be 9.87g/cm³ for the BR2 specific loading (see Appendix A).

7. Fresh matrix thermal properties (beryllium)

Beryllium used in nuclear reaction is never 100% pure and contains a certain amount of impurities and a small percentage of BeO. The exact composition of the BR2 beryllium is unknown at this moment.

7.1 Thermal conductivity

The thermal conductivity of 216 W/m-K [12] for pure beryllium is consistent with the reported thermal conductivity near room temperature for unirradiated TE-56 beryllium [13]. The thermal conductivity dependence on temperature is the strongest for unirradiated beryllium [13]. Eq. 11 is extracted from the proposed trend line to represent the unirradiated TE-56 beryllium thermal conductivity (in W/m-K) variation as a function of temperature in Ref. [13].

$$k_t = 242.36 - 0.2965 T, \quad (11)$$

where T is the temperature in °C.

However, for unirradiated TE-400 beryllium grade, Eq. 12 represents the change in thermal conductivity with temperature.

$$k_t = 194.31 - 0.2254 T, \quad (12)$$

where T is the temperature in °C.

At 200°C, the thermal conductivities are 183 W/m-K for the TE-56 beryllium and 149 W/m-K for the TE-400 beryllium.

Until more information is available on the BR2 specific beryllium, it is proposed that the more conservative value of 149 W/m-K be used as temperature-independent thermal conductivity for fresh beryllium. Tabulated values as a function of temperatures are given in Table 4.

7.2 Specific heat capacity

A specific heat capacity of 1.925 J/g-K [12] will be assumed.

7.3 Density

The minimum bulk density of beryllium depends on the weight percent of BeO. Eq. 13 can be used to evaluate the density assuming a 1% fabrication porosity [16].

$$\rho_{Be} = 0.99 \times \frac{100}{\frac{100 - \%[BeO]}{1.8477} + \frac{\%[BeO]}{3.009}} \quad (13)$$

Assuming a 1 w/o of BeO, the density of the beryllium matrix is 1.836 g/cm³.

8. Fuel channel extensions and other structures (stainless steel)

The exact composition of the stainless steel alloy used in lower and upper extensions of the BR2 channels is not known at this point. Therefore, thermal properties for stainless steel alloy 304 will be assumed.

8.1 Thermal conductivity

According to Ref. [10], the thermal conductivity of stainless steel alloy 304 is 16.2 W/m-K in the range of 0 to 100°C and 21.5 W/m-K at 500°C. It is proposed that 16.2 W/m-K be used as the temperature-independent thermal conductivity of stainless steel.

8.2 Specific heat capacity

Ref. [10] indicates that the stainless steel 304 alloy has a specific heat capacity of 0.500 J/g-K in the range of 0 to 100°C.

8.3 Density

The density of the stainless steel alloy 304 is 8.0 g/cm³ [10].

9. Thermal properties after irradiation

In a BR2 HEU fuel assembly, the maximum heat flux of 470 W/cm² (see Appendix B) is obtained at an average fuel burnup above 15% at ²³⁵U. The heat flux remains high (above 450 W/cm²) until the average burnup reach about 25% at ²³⁵U [21].

It can be seen from Eqs (1) and (2) that the thermal conductivity of the meat degrades with irradiation through the creation of a reaction-product phase as well as porosity from fission gas.

Considering that the BR2 fuel assembly heat flux remains high at relatively large burnup, it is necessary to determine thermal properties for depleted fuel to ensure that the fuel meat is not challenged.

To be conservative, it will be assumed that the maximum heat flux (470 W/cm^2) in an HEU fuel assembly is reached at 25%at ^{235}U in average burnup. Assuming a power peak-to-average ratio of 1.2, a peak burnup of 30%at of ^{235}U is calculated. This corresponds to a cumulative fission density of about $7.8\text{E}20 \text{ fission/cm}^3$. This value is used to evaluate the fuel meat thermal properties.

9.1 UAl_x fuel meat

According to Ref. [22], the total change in volume of the UAl_x-Al fuel is between 0.12%/at U burnup and 0.23%/at U burnup. It can be approximated that the swelling results equally from change in volume due to the solid and gaseous fission products [9, [23, [24]. Therefore, half of the total swelling (attributed to gaseous fission products) is used in determining the porosity. Assuming a peak total U burnup of about 24%at in the BR2 HEU fuel assembly, the porosity is estimated to be between 1.5% and 3%.

For the uranium loadings studied in Ref. [22], the volume fraction of the dispersed phase and reaction-product phase (UAl₃ reacted and transformed to UAl₄) increases from 29% at 0% burnup up to about 40% at 30% burnup. Using these assumptions in Eq. 1, the thermal conductivity of the UAl_x-Al degrades from 113 W/m-K at 0% burnup to 97 W/m-K at 30% peak burnup (i.e., a 16.5% decrease). It is therefore proposed that the conservative value of 80 W/m-K previously selected be also decreased by 16.5% to 69 W/m-K.

The revised method for calculating the thermal conductivity of irradiated HEU fuel meat is given in Appendix B.

9.2 U-7Mo fuel meat thermal conductivity

For U-7Mo-Al fuel meat, Ref. [24] indicates that the volume fraction of the reaction-product phase can be estimated using the following equation.

$$Y^2 = A F_r^{0.5} \exp\left(-\frac{Q}{RT} - \alpha W_{si} - \beta W_{si}^2\right) t \quad (14)$$

where Y is the diffusion layer thickness in cm, A , Q , α and β are correlation constants, F_r is the fission rate in the fuel particles in fission/cm³-s, R is the gas constant in cal/mol-K, T is the fuel temperature in K, W_{si} is the weight percent of silicon in the matrix, and t is the irradiation time in seconds.

Using Eq 14 and typical BR2 operating conditions at the hot spot, the volume fraction of the reaction-product phase can be estimated to be between 10%-16% for 4-5 weight % of Si in the

matrix. Given the results of the most recent irradiation experiment, E-Future, E-Future II and Selenium, a larger Si content, a fuel particle coating or other non-identified solution will be used which will reduce the volume fraction of the reaction-product phase. However, at this point, the more conservative values discussed here will be used.

Therefore the total volume fraction of the reaction-product and fuel particle would be between 59% and 65%. Assuming a well behaved U-7Mo fuel (with Si added) irradiated up to 2.1×10^{21} fission/cm³, the porosity from the fission gas is estimated to be between 2%-4% [9].

Using the above information, the degraded thermal conductivity is estimated to be between 41 and 53 W/m-K at the location of the peak burnup. According to Ref. [18], the fuel meat temperature remains rather insensitive to the degradation of the thermal conductivity until it reaches about 25 W/m-K.

In the case of BR2, when the burnup is sufficiently high to degrade the thermal conductivity below 25 W/m-K, the maximum heat flux is significantly reduced so that this degradation should not be a safety concern.

It is therefore proposed that a temperature-independent thermal conductivity of 41 W/m-K be assumed for irradiated fuel.

The revised method for calculating the thermal conductivity of irradiated LEU fuel meat is given in Appendix B.

9.3 Beryllium

Ref. [13] shows that depending on the grade of beryllium the thermal conductivity can degrade significantly under irradiation, i.e., reduced by a factor 4. Considering that the thermal conductivity remains relatively large after degradation (near 50 W/m-K after really long irradiation) and since the beryllium is cooled by coolant in the fuel channel and the bypass flow in the interstices between hexagons, this is not believed to be a safety concern. It is proposed that for irradiated beryllium, 50 W/m-K be used as a temperature-independent thermal conductivity.

References

- [1] David Plancq, Private Communication, CEA-Cadarache, France (2002).
- [2] MatWeb website,
<http://www.matweb.com/search/datasheet.aspx?MatGUID=0cd1edf33ac145ee93a0aa6fc666c0e0>.
- [3] M. E. Cunningham and K. L. Peddicord, "Heat Conduction in Spheres Packed in an Infinite Regular Cubical Array," International Journal of Heat and Mass Transfer, Vol. 24 (1981) pp. 1081-1088.
- [4] A. Beeckmans, "Influence du passage d'eau entre plaques combustibles sur le flux de chaleur maximum admissible au réacteur BR2", SCK, Dept. BR2, R0616, R0586 (Le 17 Mars, 1986).
- [5] MatWeb website,
<http://www.matweb.com/search/DataSheet.aspx?MatGUID=c71186d128cd423d9c6d51106c015e8f&ckck=1>
- [6] IAEA-TECDOC-643 Volume 4: Fuels, Appendix I-1.1, IAEA, April 1992.
- [7] Y. S. Kim, Private communication, October 25th, 2010.
- [8] Y.S. Touloukian, Thermophysical Properties of Materials, IFI/Plenum, 1975.
- [9] U-Mo Fuels Handbook. ANL-09/31 Version 1.0. Compiled by J. Rest, Y. S. Kim, G. L. Hofman ANL and M.K. Meyer and S. L. Hayes, INL. RERTR-ANL, ANL-09/31, June 2006.
- [10] MatWeb website,
<http://www.matweb.com/search/datasheet.aspx?MatGUID=abc4415b0f8b490387e3c922237098da>
- [11] MatWeb url,
<http://www.matweb.com/search/DataSheet.aspx?MatGUID=1b8c06d0ca7c456694c7777d9e10be5b&ckck=1>
- [12] MatWeb url,
<http://www.matweb.com/search/DataSheet.aspx?MatGUID=8a6a0df6122349b7bdc92662658d4a4f>
- [13] Syslov, D. N., Chakin, V. P., and Latypov, R.N., "Influence of high dose neutron irradiation of thermal conductivity of beryllium," Journal of Nuclear Materials, 307-311 (2002) 664-667.
- [14] Copeland, G.L., Hobbs, R.W., Hofman, G.L., Snelgrove, J.L., "Performance of low-enriched U3Si2-aluminum dispersion fuel assemblies in the Oak Ridge Research Reactor," ANL/RERTR/TM-10, 1987.

- [15] Web URL,
<http://www.matweb.com/search/DataSheet.aspx?MatGUID=bb191b05a9424da5bdef4be5cad33182>
- [16] “Volume 4 – Veiligheidsevaluatie,” Reactor BR2 Beschrijving en veiligheidsdossier, SCK-CEN, Dossier 72. S 7680.
- [17] G.L. Hofman and M.K. Meyer, “Properties of U–Mo Alloy Dispersion Fuel,” IAEA Technical Meeting on the Development of High Density Uranium–Molybdenum Dispersion Fuel, Vienna, Austria, Jun. 23-25, 2003.
- [18] Medvedev, P.G., “Effect of In-pile Degradation of the Meat Thermal Conductivity on the Maximum Temperature of the Plate-type U-Mo Dispersion Fuels,” Proceedings of the 31st RERTR Meeting on Reduced Enrichment for Research and Test Reactors, Beijing, China, 2009.
- [19] Y.S. Touloukian et al, Thermal conductivity, IFI, 1970.
- [20] I. Barin, Thermochemical Data of Pure Substances, 3rd ed., VCH, 1989.
- [21] Koonen, E. Private communication, July 2010.
- [22] Dienst, W., Nazare, S., and Thummler, F., “Irradiation behavior of UAl_x-Al dispersion fuels for thermal high flux reactors,” Journal of Nuclear Materials, 64 (1977), 1-13.
- [23] Hofman, G, Private communication, November 2010.
- [24] Kim, Y. S., Unpublished data, Argonne national Laboratory, June 2011.
- [25] B. Dionne, A. P. Olson, M. Kalimullah, E. Feldman, C. P. Tzanos, J. G. Stevens, Argonne National Laboratory, unpublished information, 2011.
- [26] G. Van den Branden, “Conversion Studies: BR2 Reference Data Part 1: Vessel, Reactor core, Load elements”, BR2/RCE/GVdB/2011/90/Reference_data_part-ed 1, 29-09-2011.
- [27] W. Wagner and A. Pruss, The IAPWS formulation 1995 for the thermodynamic properties of ordinary water substance for general and scientific use,” J. Phys. Chem. Ref. Data 31, 387, 2002.
- [28] G. Van den Branden, Private communication, November 2014.
- [29] A. Bergeron, Private communication, October 2014.
- [30] Y.S. Kim, G.L. Hofman, A.B. Robinson, J.L. Snelfrove and N. Hanan, “Oxidation of aluminum alloy for research and test reactor fuel,” J. Nucl. Mat, 378, 2008.
- [31] Y.S. Kim and G.L. Hoffman, “Fission product induced swelling of U-Mo alloy fuel”, Journal of Nuclear Materials, 419 (2011) 291-301.
- [32] Leenaers A., Van Eyken J., Van den Berghe S., Koonen E., Charollais F., Lemoine P., e.a.- LEONIDAS E-FUTURE : Results of the Destructive Analyses of the U(Mo)-Al(Si) Fuel

Plates.- In: RRFM / IGORR 2012 Transactions, Prague, Czech Republic, 18-22 March 2012, Belgium, ENS, 2012.

- [33] M.E. Cunningham and K.L. Peddicord, "Heat Conduction in Spheres Packed in an Infinite Regular Cubical Array," Inter. J. Heat Mass Transfer, 24, 1081 (1981).
- [34] V. Marelle, F. Huet, P. Lemoine, "Thermo-Mechanical Modelling of U-Mo Fuels with MAIA," 8th Inter. Mtg. on RRFM, Munich, Germany, Mar. 21-24, 2004.
- [35] Z. Hashin and S. Shtrikman, "A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials," J. Appl. Phys., 33, 3125 (1962).

Appendices

A Volume fraction of fuel particles in meat of dispersion fuel

The methodology used to calculate the mass and volume fraction is described in details in Ref. [6]. The following equations can be used to relate the volume fraction of the dispersed phase (V_f^D) in the fuel meat to the uranium density in the fuel meat (ρ_U).

$$V_f^D = \frac{\rho_U}{w_U^D \rho_D}$$

where

$$\rho_U = \frac{(1 - P) w_U}{\frac{1}{\rho_{Al}} - a w_U} \quad w_U = \frac{\rho_U / \rho_{Al}}{(1 - P) + a \rho_U}$$

where

$$a = \frac{1}{w_U^D} \left(\frac{1}{\rho_{Al}} - \frac{1}{\rho_D} \right)$$

$$P = \text{Porosity} = \frac{\text{Volume of Voids}}{\text{Volume of Solids} + \text{Volume of Voids}}$$

w_U = Weight Fraction of Uranium in the Fuel Meat

w_U^D = Weight Fraction of Uranium in the Dispersed Phase

ρ_{Al} = Density of Aluminum = 2.7 g/cm³

ρ_D = Density of the Dispersed Phase

Table A-1 Data for UAl_x-Al meat

	Value	Unit
²³⁵ U Enrichment	93	%
Weight fraction U in fuel particle (w^D_U)	70	%
Density of Aluminum matrix (ρ_{Al})	2.70	g/cm ³
Density of dispersed phase (ρ_D)	6.36	g/cm ³
Porosity	7	%
Density of fuel meat	3.57	g/cm ³
Density U in fuel meat (ρ_U)	1.29	g/cm ³
Volume fraction of dispersed phase (V^D_f)	29	%
Mass U235 in element	400	g
Density of Al in fuel meat	2.36	g/cm ³
"a"	0.30	cm ³ /g
Weight fraction U in fuel meat (w_U)	35	%
Meat Volume/fuel assembly	331	cm ³

Table A-2 Data for U-7Mo-Al meat

	Value	Unit
²³⁵ U Enrichment	19.75	%
Weight fraction U in fuel particle (w^D_U)	93	%
Density of Aluminum matrix (ρ_{Al})	2.7	g/cm ³
Density of dispersed phase (ρ_D)	17.53	g/cm ³
Porosity	4	%
Density of fuel meat	9.87	g/cm ³
Density U in fuel meat (ρ_U)	8.00	g/cm ³
Volume fraction of dispersed phase (V^D_f)	49.07	%
Mass U235 in fuel assembly	523	g
Density of Al in fuel meat	1.87	g/cm ³
"a"	0.3369	cm ³ /g
Weight fraction U in fuel meat (w_U)	80.94	%
Meat Volume/fuel assembly	331	cm ³

B Updated methodology to determine fuel thermal conductivity

This section of the document provides the current methodology for determining the thermal conductivity values associated with the HEU and LEU fuel elements for the conversion analyses of the BR2 reactor. The analysis for the HEU fuel element was based on the current fuel element containing $\text{UAl}_x\text{-Al}$. Although the LEU fuel element was in the development phase at the time of this work, the analysis described here was based on the latest information available for the leading LEU fuel candidate (U-7Mo-Al).

The first section of this document (B.1) describes the power and burnup history that was assumed for determining the thermal conductivity of the HEU and LEU fuel element.

The second section of this document (B.2) discusses the details for the methods used in determining the thermal conductivity of LEU fuel as a function of burnup and heat flux. The calculations were divided into separate logical parts:

- B.2.1 Coolant/oxide interface temperature
- B.2.2 Oxide thickness
- B.2.3 Oxide/clad/fuel interface temperature
- B.2.4 Fuel particle swelling
- B.2.5 Interaction layer growth
- B.2.6 Volume fractions
- B.2.7 Thermal conductivity
- B.2.8 Meat temperature

The third section of this document (B.3) gives a description of the methods used to determine the HEU thermal conductivity as a function of burnup. The calculation methods are quite different from that used for LEU fuel. They are also relatively simpler and independent of the meat temperature. However, the meat temperature for HEU fuel can be determined using the same calculation methodology as LEU by replacing steps B.2.4 through B.2.7 listed above with the methods described for HEU.

The fourth section (B.4) provides the results from the calculations.

B.1 Power and burnup history

The determination of the thermal conductivity for BR2 fuel is quite complex since the burnup history of each element is different during its lifetime in the reactor. It can be assumed that a fuel element is shuffled to four locations (four cycles) throughout its lifecycle with an average BOC burnup value of 0%, 16%, 32% and 46% for each location. The actual average burnup value for a given fuel element will somewhat vary from this. For each group of fuel elements at a given cycle, there will be one fuel element that operates at a highest heat flux. At the location of the highest heat flux, there will be a local burnup value that exceeds the average of the fuel element (due to the power distribution). MCNP calculations were performed with the

representative core at BOC for both HEU and LEU fuel to obtain the heat flux values for each fuel element. Table B-1/Figure B-1 and Table B-2/Figure B-2 give the maximum heat flux found in each group of fuel elements (each average burnup value) and the associated peak local burnup value for HEU and LEU, respectively. The tables also list the channel identified in MCNP as containing the high heat flux fuel element.

Table B-1 Burnup and maximum heat flux for HEU fuel at BOC of each cycle.

Average Burnup	Maximum Heat Flux	Local Burnup	High Heat Flux Channel
0%	413 W/cm ²	0.0%	C-259 (BOC)
16%	470 W/cm ²	23.9%	A-030 (BOC)
32%	408 W/cm ²	45.6%	H1 (BOC)
46%	224 W/cm ²	59.3%	F-346 (BOC)

Figure B-1 Peak burnup for the maximum heat flux of HEU fuel for each cycle.

Table B-2 Burnup and maximum heat flux for LEU fuel at BOC of each cycle.

Average Burnup	Maximum Heat Flux	Local Burnup	High Heat Flux Channel
0%	438 W/cm ²	0.0%	C-319 (BOC)
16%	470 W/cm ²	27.2%	A-030 (BOC)
32%	415 W/cm ²	46.0%	H1 (BOC)
46%	236 W/cm ²	52.0%	F-346 (BOC)

Figure B-2 Peak burnup for the maximum heat flux of LEU fuel for each cycle.

A hypothetical fuel element has been used for the determination of the representative thermal conductivity for both an HEU and LEU fuel element. Although it is highly unlikely that a given fuel element will operate at the highest heat flux at each cycle during its lifecycle, this was the case considered for the hypothetical fuel element. Thus, it is conservatively assumed that the hypothetical fuel element used for this analysis was operated at the maximum heat flux at each cycle of its lifecycle.

It is also important to note that the heat flux values have only been determined for BOC conditions. EOC calculations are not currently available. Thus, it is conservatively assumed that the EOC conditions are equivalent to the BOC condition for the following stage to allow heat flux and burnup values to evolve continuously for these analyses. This assumption may be revisited when EOC calculations are available. The heat flux and burnup values in Figures B-1 and B-2 have been extrapolated from 90 days out to 120 days for the last cycle for illustrative purposes.

B.2 Thermal conductivity of a fuel element containing U-7Mo-Al (LEU)

The following sections (B.2.1 - B.2.8) outline the equations used to determine thermal conductivity and other relevant parameters.

B.2.1 Coolant/oxide interface temperature

The coolant/oxide interface temperature ($T_{b/o}$) was calculated with Newton's law of cooling:

$$T_{b/o} = \frac{Q''}{h} + T_b$$

where Q'' is the heat flux and T_b is bulk coolant temperature. The heat transfer coefficient (h) was defined with the Dittus-Boelter correlation:

$$h = \frac{k_b}{D_h} 0.023 Re^{0.8} Pr^{0.4}$$

and the inputs were as follows:

Table B-3 Input parameters to determine coolant/oxide interface temperature

Parameter (symbol)	Value	Reference	Parameter (symbol)	Value	Reference
Coolant temperature (T_b)	313 K	Inlet conditions [25]	Coolant density (ρ)	992.7 kg/m ³	[27]
Coolant pressure	1.24e ⁶ Pa		Coolant viscosity (μ)	6.531e ⁻⁴ kg/m-s	
Coolant velocity (V_c)	10.4 m/s	[26]	Coolant conductivity (k_b)	0.6311 W/m-K	
Channel thickness	3.00e ⁻³ m	Based on the 6 th channel in a BR2 fuel element [26]	Coolant specific heat	4177 J/kg-K	
Channel width	6.941e ⁻² m		Prandtl number(Pr)	4.322	$Re = \rho V_c D_h / \mu$
Hydraulic diameter (D_h)	5.75e ⁻³ m		Reynolds number (Re)	90901	

B.2.2 Oxide thickness

Table B-4 Input parameters, equations and assumptions to determine oxide thickness.

Parameter (symbol, unit)	Equation	Comments, Reference.
Correction factor (B)	$B = 0.022$	Correction factor for reduction in oxide thickness due to oxide migration [29].
Augmentation factor (A)	$A = 0.43 + \frac{3.21}{\left(1 + \exp\left(\frac{13.39 - V_c}{3.6}\right)\right)}$	Takes into account the effect of coolant velocity on oxide growth [30].
Oxide conductivity (k_{ox} , W/m-K)	$k_{ox} = \begin{cases} 2.25, & t_{ox} \leq 25 \\ 2.25 - 0.016(t_{ox} - 25), & 25 < t_{ox} \leq 100 \\ 1.05, & t_{ox} > 100 \end{cases}$	Assumed independent of temperature but dependent on thickness [30]. Currently limited to 45 μm [28].
Reaction constant (k)	$k = 900 \exp\left(\frac{-3800}{T_{b/o} + \frac{A \cdot B \cdot \frac{Q''}{1E8} \cdot t_{ox}}{k_{ox}}}\right)$	Modification to the reaction temperature to factor in temperature difference across oxide [29].
pH	$\text{pH} = 5.6 \pm 0.3$	Mean and uncertainty from daily measurements of BR2 during operation from 02/01/2011 through 05/13/2014 [28].
Oxide solubility (C_s)	$C_s = \exp\left(\left(\frac{1211.6}{T_{b/o}} + 13.79\right)(-0.07 - 0.41\text{pH} + 0.041\text{pH}^2)\right)$	[30]
Rate-law power (p)	$p = 0.12 + 9.22 \exp\left(\frac{-C_s}{6.82E-9}\right)$	[30]
Oxide thickness (t_{ox} , μm)	$t_{ox} = \left(t_{ox-1}^{(p+1)} + (p+1)k \cdot 24\right)^{\left(\frac{1}{p+1}\right)}$	It is assumed that 24 hour time steps correctly capture the dynamics of the phenomena. The oxide thickness is based on the previous time step (t_{ox-1}). The initial oxide thickness is chosen to be 0 [29].

B.2.3 Oxide/clad/fuel interface temperature

Table B-5 Input parameters, equations and assumptions to determine oxide/clad and clad/fuel interface temperature.

Parameter (symbol, unit)	Equation	Comments, Ref.
Initial clad thickness ($t_{c,i}$, μm)	$t_{c,i} = 381$	[26]
Clad thermal conductivity (k_c , W/m-K)	$k_c = 130$	Historically, BR2 has assumed a thermal conductivity of 150 W/m-K [4] for its cladding (AG3NE or AISI5754 alloy). The 5000 aluminum alloy series (see Ref. [9]) have thermal conductivities varying between 108 and 205 W/m-K [5] with an average of 143 W/m-K. Ref. [6] states that thermal conductivity of the AG3NE is about 130 W/m-K. It is proposed that 130 W/m-K is used as a temperature-independent thermal conductivity for the BR2 fuel cladding.
Oxide penetration into cladding (pen , %)	$pen = 40$	[29]
Clad thickness (t_c , μm)	$t_c = t_{c,i} - \frac{pen}{100} t_{ox}$	Clad thickness decreases due to consumption associated with oxide growth.
Oxide/clad interface temperature ($T_{o/c}$, K)	$T_{o/c} = T_{b/o} + \frac{t_{ox} Q''}{k_{ox}} \cdot \left(\frac{10000 \text{ cm}^2/\text{m}^2}{1000000 \mu\text{m}/\text{m}} \right)$	Fourier's law with unit conversion factor.
Clad/fuel interface temperature ($T_{c/f}$, K)	$T_{c/f} = T_{o/c} + \frac{t_c Q''}{k_c} \cdot \left(\frac{10000 \text{ cm}^2/\text{m}^2}{1000000 \mu\text{m}/\text{m}} \right)$	Fourier's law with unit conversion factor.

B.2.4 Fuel particle swelling

Table B-6 Input parameters, equations and assumptions to determine fuel particle swelling.

Parameter (symbol, unit)	Equation	Comments, Ref.
Initial fuel volume fraction ($V_{f,fp,i}$)	$V_{f,fp,i} = 0.49$	Appendix A
^{235}U atomic density (ρ_{U235} , at/cc _{of_fuel_kernal})	$\rho_{U235} = \frac{8 \cdot 6.022e^{23} \cdot 0.1975}{235V_{f,fp,i}}$	Assumptions: U-7Mo density = 8gU/cm ³ and ^{235}U enrichment = 19.75%.
Fission density (f_d , fission/cc _{of_fuel_kernal})	$f_d = \rho_{U235} \frac{BU}{100}$	Assume ^{235}U burnup is directly converted into fission density (conservative).
Fuel particle swelling (S_{fp} , %)	$S_{fp} = \begin{cases} f_d \cdot 5e^{-21}, & f_d < 3e^{21} \\ 15 + (f_d - 3e^{21})6.3e^{-21} + 0.33(f_d \cdot 1e^{-21} - 3)^2, & f_d \geq 3e^{21} \end{cases}$	[31]
Fuel particle porosity (P_{fp} , %)	$P_{fp} = S_{fp} - f_d 5e^{-21}$	Deviation in fuel particle swelling from linear rate due to gas bubble formation and growth (porosity) [31].

B.2.5 Interaction layer growth

There are a number of equations and assumption used in determining the interaction layer growth so a brief description of the logic is given here. An important assumption in determining the fuel particle, interaction layer and matrix volumes is that the fuel particles are dispersed in the matrix with an FCC crystallographic structure. The size of the FCC structure was based on the fuel particle radius and volume fraction at beginning of life conditions. The fuel swelling was used to determine the change in FCC structure size and fuel particle radius with burnup. It was also assumed that the swelling only occurs in one direction (direction of plate thickness). A correlation was used to determine interaction layer growth as function of burnup. From a calculation point of view, the growths of the fuel particle and interaction layer were assumed to be unimpeded. However, when the thickness of the interaction layer (t_{IL}) was large enough that neighboring particles intersected, the intersecting volume (V_{cap1} and V_{cap2}) was removed from the total interaction layer volume. The total volume of the FCC structure (V_{FCC}) was conserved (not including volume change due to swelling) such that the growth of the interaction layer volume (V_{IL}) resulted in a decrease in the matrix volume (V_m).

Figure B-3 Description of the variables used in the calculations associated with the interaction layer growth.

Table B-7 Input parameters, equations and assumptions to determine interaction layer growth.

Parameter (symbol, unit)	Equation	Comments, References
Fission rate (f_r , f/cc _{of_fuel_kernal} /s)	$f_r = \frac{(f_d - f_{d-1})}{24 \cdot 3600}$	Change in fission density divided by change in time (1 day).
Silicon weight fraction (w_{Si} , %)	$w_{Si} = 4$	4% and 6% silicon has been used in the E-FUTURE tests [32]. 4% has been chosen to be conservative.
Molybdenum weight fraction (w_{Mo} , %)	$w_{Mo} = 7$	U-7Mo-Al dispersion fuel is current reference LEU fuel.
Initial radius of fuel particle ($r_{fp,i}$, μm)	$r_{fp,i} = 30$	[29]
Initial volume of fuel in FCC ($V_{fp,i}$, μm^3)	$V_{fp,i} = \frac{16\pi}{3} r_{fp,i}^3$	It was assumed the fuel particles are distributed in an FCC lattice. There are 4 fuel particles in an FCC lattice.
Initial volume of FCC ($V_{FCC,i}$, μm^3)	$V_{FCC,i} = \frac{V_{fp,i}}{V_{f,fp,i}}$	
Initial matrix volume ($V_{m,i}$, μm^3)	$V_{m,i} = V_{FCC,i} - V_{fp,i}$	
Initial FCC unit edge, (l_i , μm)	$l_i = \sqrt[3]{V_{FCC,i}}$	
(initial) Half the distance between fuel particle centers (d_i , μm)	$d_i = \frac{l_i}{2\sqrt{2}}$	Half the distance between particle centers in FCC lattice.
Radius of fuel particle (r_{fp} , μm)	$r_{fp} = \left(V_{fp,i} (1 + S_{fp}/100) \frac{3\pi}{16} \right)^{1/3}$	Radius of fuel particle including swelling. Volume based on four fuel particles.

Volume of fuel in FCC (V_{fp} , μm^3)	$V_{fp} = 4 \frac{4}{3} \pi r_{fp}^3$	Volume of four fuel particles
Volume of FCC (V_{FCC} , μm^3)	$V_{FCC} = V_{m,i} + V_{fp,i} \left(1 + \frac{S_{fp}}{100} \right)$	Original volumes, fuel particle volume includes modifier for swelling.
FCC unit edge (l , μm)	$l = \frac{V_{FCC}}{l_i^2}$	Calculation assumes two directions are fixed in dimension and swelling occurs in the third dimension (direction associated with meat thickness).
Half the distance between fuel particle centers (d , μm)	$d = \frac{1}{2} \sqrt{\frac{l_i^2}{4} + \frac{l^2}{4}}$	Calculation assumes two directions are fixed in dimension and swelling occurs in the third dimension (direction associated with meat thickness).
Interaction layer thickness (t_{IL} , μm)	$t_{IL} = \sqrt{t_{IL-1}^2 + 2.6e^{-8} f_r^{0.5} e^{\left(\frac{-3850}{T_{meat}} - 0.69w_{Si} - 0.043w_{Si} \right)} \cdot 1 \cdot 24 \cdot 3600}$	Thickness = 0 at 0 BU, all other BU values references previous thickness value (t_{IL-1}). (T_{meat} defined in B.2.8) Equation reference: [29]
Radius of fuel particle and interaction layer (r_{fp+IL} , μm)	$r_{fp+IL} = r_{fp} + t_{IL}$	Fuel particle radius plus interaction layer thickness.
Height of spherical cap (h_1 , μm)	$h_1 = \begin{cases} 0, & r_{fp+IL} - d_i < 0 \\ r_{fp+IL} - d_i, & r_{fp+IL} - d_i \geq 0 \end{cases}$	This represents the radius of the fuel particle sphere that extends beyond the intersection of the neighboring particle surface. This calculation is based on the width direction and is based on d_i

Height of spherical cap (h_2 , μm)	$h_2 = \begin{cases} 0, & r_{fp+IL} - d < 0 \\ r_{fp+IL} - d, & r_{fp+IL} - d \geq 0 \end{cases}$	This represents the radius of the fuel particle sphere that extends beyond the intersection of the neighboring particle surface. This calculation is based on the thickness direction and is based on d
Base of the spherical cap (a_1 , μm)	$a_1 = \begin{cases} 0, & h_1 = 0 \\ \sqrt{(r_{fp+IL}^2 - (r_{fp+IL} - h_1)^2)}, & h_1 \neq 0 \end{cases}$	This represents the height of the fuel particle sphere that is associated with the intersection of the neighboring particle surface. This calculation is based on the width direction and is based on h_1
Base of the spherical cap (a_2 , μm)	$a_2 = \begin{cases} 0, & h_2 = 0 \\ \sqrt{(r_{fp+IL}^2 - (r_{fp+IL} - h_2)^2)}, & h_2 \neq 0 \end{cases}$	This represents the height of the fuel particle sphere that is associated with the intersection of the neighboring particle surface. This calculation is based on the thickness direction and is based on h_2
Volume of spherical cap (V_{cap1} , μm^3)	$V_{cap1} = \frac{\pi h_1}{6} (3a_1^2 + h_1^2)$	This is the intersection volume of two spheres with a separation distance that does not include swelling.
Volume of spherical cap (V_{cap2} , μm^3)	$V_{cap2} = \frac{\pi h_2}{6} (3a_2^2 + h_2^2)$	This is the intersection volume of two spheres with a separation distance that includes swelling.
Logic1	$4 \left(\frac{4}{3} \pi (r_{fp+IL}^3 - r_{fp}^3) - 4V_{cap1} - 8V_{cap2} \right) > V_{m,i}$	$4 V_{cap1}$ is the total intersection volume due to the 2 faces in the FCC structure that do not include swelling, $8 V_{cap2}$ is the total intersection volume due to the 4 faces in the FCC structure that include swelling. Statement true if interaction layer

		volume greater than matrix volume.
Logic2	$4 \left(\frac{4}{3} \pi (r_{fp+IL}^3 - r_{fp}^3) - 4V_{cap1} - 8V_{cap2} \right) < 0$	4 V_{cap1} is the total intersection volume due to the 2 faces in the FCC structure that do not include swelling, 8 V_{cap2} is the total intersection volume due to the 4 faces in the FCC structure that include swelling. Statement true if interaction layer volume less than 0.
Volume of interaction layer (V_{IL} , μm^3)	$V_{IL} = \begin{cases} V_{m,i}, & \text{Logic1 or Logic2} = \text{true} \\ 4 \left(\frac{4}{3} \pi (r_{fp+IL}^3 - r_{fp}^3) - 4V_{cap1} - 8V_{cap2} \right), & \text{Logic1 and Logic2} = \text{false} \end{cases}$	If logic1 or logic 2 is true, interaction layer volume is equal to matrix volume. Otherwise interaction layer volume is calculated.
Matrix Volume (V_m , μm^3)	$V_m = V_{m,i} - V_{IL}$	Difference of initial matrix volume and interaction layer volume.

B.2.6 Volume fractions

The fuel, matrix and interaction layer volume fractions were determined from the following equations:

Fuel volume fraction ($V_{f,fp}$): $V_{f,fp} = \frac{V_{fp}}{V_{FCC}}$

Matrix volume fraction ($V_{f,m}$): $V_{f,m} = \frac{V_m}{V_{FCC}}$

Interaction layer volume fraction ($V_{f,IL}$): $V_{f,IL} = \frac{V_{IL}}{V_{FCC}}$

B.2.7 Thermal Conductivity

Table B-8 Input parameters, equations and assumptions to determine LEU thermal conductivity.

Parameter (symbol, unit)	Equation	Comments, Ref.
Initial thermal conductivity of interaction layer (k_{IL} , W/m-K)	$k_{IL} = 16$	Assumed conductivity of interaction layer.
Initial thermal conductivity of matrix (k_m , W/m-K)	$k_m = 210$	For the aluminum matrix of both fuels (pure aluminum), a thermal conductivity of 210 W/m-K is reported in Ref. [2]. Ref. [19] reports a thermal conductivity closer to 240 W/m-K near room temperature which decreases near around 210 W/m-K near the melting point. It was assumed that the fuel meat thermal properties use 210 W/m-K as a temperature independent thermal conductivity for aluminum matrix.
Initial thermal conductivity of fuel particle (k_{UMo} , W/m-K)	$k_{UMo} = 16$	
Thermal conductivity of UMo (k_{UMo} , W/m-K)	$k_{UMo} = (2.2 + 0.032T_{meat}) \exp \frac{-2.14P_{fp}}{100}$	Includes porosity effect by including decay factor given by Ref: [33].
Thermal conductivity of UMo and interaction layer (k_{UMo-IL} , W/m-K)	$\frac{k_{umo-IL}}{1} = \frac{1}{\frac{1}{k_{UMo}} \left(1 - \frac{t_{IL}}{t_{IL} + r_{fp,i}}\right) + \frac{1}{k_{IL}} \left(\frac{t_{IL}}{t_{IL} + r_{fp,i}}\right)}$	This equation describes the thermal conductivity of materials in series. Assumes thickness of interaction layer is thin relative to radiuses so that equation for flat plates in series has sufficient accuracy [34].
Bruggeman constant (A_B)	$A_B = \frac{(3(V_{f,fp} + V_{f,IL}) - 1)k_{UMo-IL} + (3V_{f,m} - 1)k_m}{4}$	[34][35]
Thermal conductivity meat (k_{meat} , W/m-K)	$k_{meat} = \frac{A_B + \sqrt{8k_{umo-IL}k_m + A_B^2}}{4}$	[34][35]

B.2.8 Meat temperature

Table B-9 Input parameters, equations and assumptions to determine meat centerline temperature.

Parameter (symbol, units)	Equation	Comments, Ref.
Initial meat thickness ($t_{meat,i}$, μm)	$t_{meat,i} = 508$	Standard fuel meat thickness [26]
Meat thickness (t_{meat} , μm)	$t_{meat} = t_{meat,i}(1 - V_{f,fp,i}) + t_{meat,i}V_{f,fp,i}\left(1 + \frac{S_{fp}}{100}\right)$	Non fuel thickness plus fuel thickness (initial fuel thickness plus swelling component)
Centerline meat temperature (T_{meat} , K)	$T_{meat} = T_{meat/clad} + \frac{t_{meat}/2}{k_{meat}} Q'' \cdot \left(\frac{10000 \text{ cm}^2/\text{m}^2}{1000000 \text{ }\mu\text{m}/\text{m}} \right)$	Fourier's law with unit conversion factor

B.3 Thermal conductivity of a fuel element containing UAl_x-Al (HEU)

The thermal conductivity of HEU dispersion fuel meat (k_{meat}) was based on Ref. [1] with the addition of a correction factor (C_1):

$$k_{meat} = \frac{-k_{fp} + 3Vk_{fp} + 2k_m - 3Vk_m + \sqrt{8k_{fp}k_m + (k_{fp} - 3Vk_{fp} - 2k_m + 3Vk_m)^2}}{4} \cdot C_1$$

Below is a description of the variables.

Composite thermal conductivity of fuel particle and reaction-product phase (k_{fp}):

$$k_{fp} = k_{fp,100}e^{-2.14P}$$

This parameter is a function of the thermal conductivity of the fuel particle and reaction-product phase at 100% density ($k_{fp,100}$) and the porosity (P).

Porosity (P):

A typical as manufactured porosity has historically been assumed to be 7% [6]. This value is known to decrease with irradiation but has been conservatively assumed constant for these analyses. Porosity also occurs due to irradiation. According to Ref [22], the total change in volume of UAl_x-Al is between 0.12%/at U burnup and 0.23%/at U burnup. It can be approximated that the swelling results equally from change in volume due to solid and gaseous fission products [9, [23, [24]. Thus, the total porosity is assumed to be the greater of the two values:

$$P = \begin{cases} 0.07, & P \leq 0.07 \\ 0.23BU/2, & P > 0.07 \end{cases}$$

Composite thermal conductivity of fuel particle and reaction-product phase at 100% density ($k_{fp,100}$):

$$k_{fp,100} = 2.17 - 2.76w$$

where w is the weight fraction of U in the alloy. For fuel containing 60% UAl₃ and 40% UAl₄ (weight fraction of 0.744 and 0.64, respectively [6]), the weight fraction is calculated to be 0.70.

Thermal conductivity of Al matrix (k_m):

$$k_m = k_{m,100}e^{-2.14P}$$

This parameter is a function of the thermal conductivity of the fuel particle and reaction-product phase at 100% density ($k_{fp,100}$) and the porosity (P).

The thermal conductivity of aluminum at 100% density ($k_{m,100}$) was assumed to be 210 W/m-K.

Volume fraction of fuel particle and reaction-product (V):

The volume fraction (V) for uranium loadings studied in Ref. [22] increases from 29% at 0% burnup to 40% at 30% burnup. From this it was assumed that the volume fraction (V) was:

$$V = 0.29 + 0.367BU$$

Correction Factor (C_1):

It is conservatively assumed that the thermal conductivity of fresh HEU fuel (BU=0) be equal to the BR2 historical value of 80 W/m-K [4]. To achieve this, k_{meat} has been multiplied by $C_1 = 0.68$

B.4 Results

The equations described in sections B.2 and B.3 were evaluated with the heat flux and burnup profiles described in section B.1. Figure B-4 shows the results for the thermal conductivity of the meat for HEU and LEU fuel.

Figure B-4 Evolution of meat conductivity for HEU and LEU.

Tables B-10 and B-11 shows additional parameters at BOC for each of the high heat flux elements for each cycle of its lifecycle.

Table B-10 Plate parameters for HEU fuel.

Element, channel	Meat thickness	Clad thickness	Oxide thickness	Plate thickness	Meat conductivity	Crud resistance
	μm	μm	μm	μm	W/m-K	$\text{m}^2\text{-K/W}$
Fresh fuel, C-259	508.0	381.0	0.0	1270.0	80.5	0
High heat flux, A-30	536.0	376.7	10.7	1310.8	64.1	4.8e-6
High power, H1	561.2	375.2	14.4	1340.5	51.2	6.4e-6
High burnup, F-346	577.3	375.1	14.9	1357.2	43.9	6.6e-6

Table B-11 Plate parameters for LEU fuel.

Element, channel	Meat thickness	Clad thickness	Oxide thickness	Plate thickness	Meat conductivity	Crud resistance
	μm	μm	μm	μm	W/m-K	$\text{m}^2\text{-K/W}$
Fresh fuel, C-319	508.0	381.0	0.0	1270.0	86.1	0
High heat flux, A-30	536.0	376.5	11.3	1311.6	36.0	5.0e-6
High power, H1	558.4	375.0	15.0	1338.5	23.5	6.7e-6
High burnup, F-346	567.0	374.8	15.6	1347.7	19.4	6.9e-6

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