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

Revision 0

Nuclear Engineering Division

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May 23, 2011

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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. This section is regrouping all of the thermal property tables.

Section 2 provides a summary of the thermal properties in form of tables while the following sections 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 (UAlx-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 shows the evolution of the BR2 maximum heat flux with burnup.

2. Thermal properties summary tables

Table 1 shows the proposed conservative temperature-independent values of the thermal properties for used in the BR2.

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	ρ C_p (J/m^3-K)
AG3NE cladding	130	880	2670	2349600
Al 6061-T6	167	896	2700	2419200
UAl$_x$-Al dispersion (fresh)	80	646	3580	2312366
U-7Mo-Al dispersion (fresh)	66	275	9870	2714250
UAl$_x$-Al dispersion (β^*=25%)	69	-	-	-
U-7Mo-Al dispersion (β=25%)	41	-	-	-
Beryllium (unirradiated)	149	1925	1836	3534300
Beryllium (long irradiation)	50	-	-	-
Stainless steel 304	16	500	8000	4000000

* 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 (UAl$_x$-Al).

Table 2 Tabulated volumetric heat capacity for BR2 fresh HEU fuel meat (UAl$_x$-Al)

Temperature		$\rho\, C_p$
°C	K	(J/m^3-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
°C	K	(W/m-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
°C	K	(W/m-K)
20	293.15	190
50	323.15	183
100	373.15	172
150	423.15	161
200	473.15	149

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 meant 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 following formula:

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

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

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

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),

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

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

4.3. Density

The density of pure aluminum is reported as 2.6989 g/cm^3 [2]. For AG3NE (aluminum alloy 5754), the density is reported as 2.67 g/cm^3 [15]. For the aluminum alloy 6061, the density is reported as 2.7 g/cm^3 [11].

5. Fresh HEU fuel meat thermal properties (UAl$_x$-Al)

The current HEU fuel (UAl$_x$) is composed mainly of UAl$_3$ and UAl$_4$ dispersed in aluminum with a ratio of typically 60% and 40%, respectively [6]. The typical loading in a HEU BR2 fuel assembly (400g of ^{235}U) requires a fuel meat density of 1.3 gU/cm^3. 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 29.09% (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,

$$k_t = 2.17 - 2.76\ w, \tag{4}$$

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

Then, assuming a value of 0.72 for w (calculated for an equivalent fuel particle made of 60% UAl$_3$ and 40% UAl$_4$), 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 Fig. 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.

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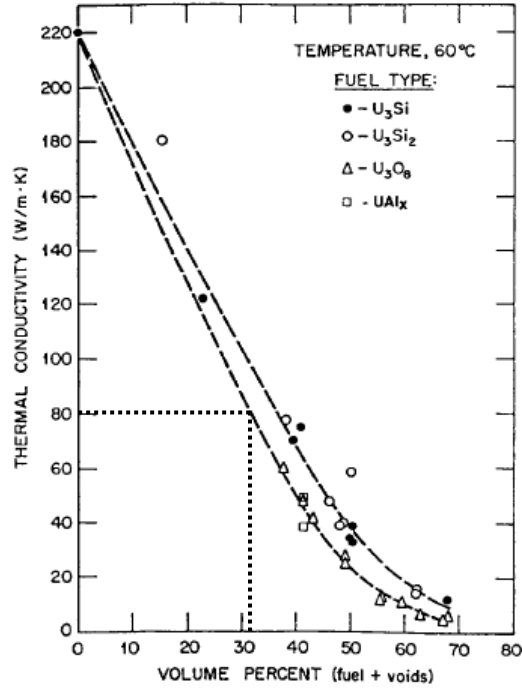
Figure 1. Thermal conductivity vs volume percent of fuel and porosity [6].

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,

$$C_{p,UAl3} = 0.329 + 0.00021\ T, \tag{5}$$

$$C_{p,UAl4} = 0.473 + 0.00024\ T, \tag{6}$$

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

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

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 ($w_{leu\ fuel}$). 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

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

where T is the temperature in K.

A slightly different relationship is presented in Ref. 17,

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

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 in calculated and given in Table 3.

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].

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

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).

6.3. Density

The U-7Mo-Al fuel meat density is calculated to be 9.87g/cm^3 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.

$$k_t = 242.36 - 0.2965\ T, \tag{11}$$

where T is the temperature in °C.

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

$$k_t = 194.31 - 0.2254\ T, \tag{12}$$

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].

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

Assuming a 1 w/o of BeO, the density of the beryllium matrix is 1.836 g/cm^3.

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/cm^3 [10].

9. Thermal properties after irradiation

In a BR2 HEU fuel assembly, the maximum heat flux of 470 W/cm^2 (see Apeendix B) is obtained at an average fuel burnup above 15%at in ^{235}U. The heat flux remains high (above 450 W/cm^2) until the average burnup reach about 25%at of ^{235}U [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 7.8E20 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 (UAl$_3$ reacted and transformed to UAl$_4$) 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.

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.

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

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 fiss/cm^3-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, a larger Si content 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 7.8E20 fission/cm^3, 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

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.

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Appendix 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^D_f) in the fuel meat to the uranium density in the fuel meat (ρ_U).

$$V^D_f = \frac{\rho_U}{w^D_U \, \rho_D}$$

where

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

where

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

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

w_U = Weight Fraction of Uranium in the Fuel Meat

w^D_U = Weight Fraction of Uranium in the Dispersed Phase

ρ_{Al} = Density of Aluminum = 2.7 g/cm^3

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)	70.24	%
Density of Aluminum matrix (ρ_{Al})	2.7	g/cm^3
Density of dispersed phase (ρ_D)	6.36	g/cm^3
Porosity	4	%
Density of fuel meat	3.66	g/cm^3
Density U in fuel meat (ρ_U)	1.3	g/cm^3
Volume fraction of dispersed phase (V^D_f)	29.09	%
Mass U235 in element	400	g
Density of Al in fuel meat	2.357	g/cm^3
"a"	0.30344	cm^3/g
Weight fraction U in fuel meat (w_U)	35.54%	%
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"	0.33691	cm^3/g
Weight fraction U in fuel meat (w_U)	80.94%	%
Meat Volume/fuel assembly	331	cm^3

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