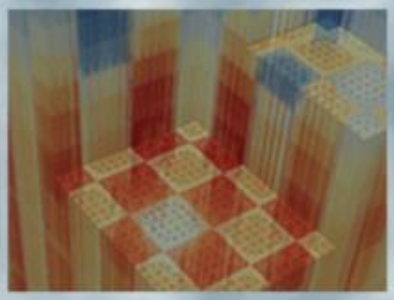
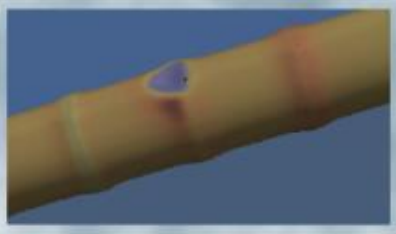
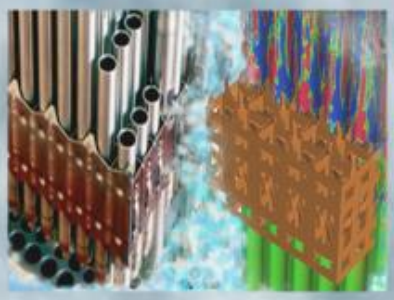
CASL-U-2016-1015-000







Investigation of Thermal Expansion Effects in MPACT

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CONTENTS

CONTENTS iii

FIGURES iv

TABLES v

ACRONYMS vi

1. Introduction 1

2. Thermal Expansion Theory 1

3. Materials 2
   3.1 Zirconium 2
   3.2. Stainless Steel 3
   3.3 Pyrex 4
   3.4 Boron Carbide (B_4C) 4
   3.5 AIC4
   3.6 Uranium dioxide 5
      3.6.1 Discussion 5
   3.7 Material Summary 6

4. Example 7
   4.1 Single Assembly Example 7
   4.2 Axial Expansion 9
   4.3 Absorber Materials 9

5. Results 10
   5.1 Pincells (BOL) 10
   5.2 2D Assemblies (BOL) 12
   5.3 Sensititivies (BOL) 13
   5.4 2D Assemblies (Depletion) 14
   5.5 3D Assemblies 17
   5.6 2D Assemblies (ITC) 18

6. Implementation Requirements 19

7. Conclusions 22

8. References 23

FIGURES

Figure 3.1: Thermal Expansion Coefficient of Pyrex [Mogulkoc Fig. 7] 4

Figure 3.2: Pellet Volume versus burnup 6

Figure 5.1: High thermal expansion results vs. depletion.....15

Figure 5.2: Nominal thermal expansion results vs. depletion.....15

Figure 5.3: Low thermal expansion results vs. depletion 16

TABLES

Table 3-1: Material Properties for SS304 3

Table 3-2: Material Summary 6

Table 5-1: Pincell Differences with Thermal Expansion (pcm) 11

Table 5-2: Assembly Eigenvalue Differences with Thermal Expansion (pcm) 12

Table 5-3: Assembly Pin Power Differences with Thermal Expansion 12

Table 5-4: Eigenvalue Results of Temperature Perturbations (pcm) 13

Table 5-6: Thermal Expansion Results for 3D Assembly 17

Table 5-7: ITC Results 18

ACRONYMS

BWR	boiling water reactor
CASL	Consortium for Advanced Simulation of Light Water Reactors
CZP	Cold Zero Power
HFP	Hot Full Power
HZP	Hot Zero Power
GT	guide tube
IT	instrument tube
ITC	isothermal temperature coefficient
LEF	linear expansion factor
LWR	light water reactor
PCM	percent mille (10^{-5})
PPM	parts per million (usually boron concentration)
PWR	pressurized water reactor
TE	thermal expansion
V&V	verification and validation
VERA	Virtual Environment for Reactor Applications

1. INTRODUCTION

The thermal expansion of materials is not currently being modeled in MPACT. Since reactor dimensions are entered at room temperature, and reactors operate at elevated temperatures, the effect of thermal expansion on the reactor materials has the potential to impact the results. This report summarizes the investigation of modeling the effects of thermal expansion in MPACT.

The first part of the report gives the theory of thermal expansion and the results of a literature review to develop a set of recommended thermal expansion coefficients to be used in MPACT.

The second part of this report looks at the effect of including thermal expansion on several test problems on MPACT results.

Finally, a set of recommendations is made to implement the thermal expansion models in MPACT.

2. THERMAL EXPANSION THEORY

For isotropic materials, the thermal expansion (TE) of a material in any direction is given by:

$$\Delta L = \alpha_L \, L_0 \, \Delta T$$

where

- α_L is the coefficient of linear thermal expansion
- L_o is the initial length (at some reference temperature)
- ΔT is the change in temperature from the reference temperature.

For materials of interest in a reactor, α_L is on the order of 5×10^{-6}/K and is usually a function of temperature. For large changes in temperatures, the coefficient must be integrated over the range of temperature change.

For cases where α_L is changing, it is often easier to consider the total change in linear dimension:

$$\frac{\Delta L}{L} = \frac{L - L_o}{L_o} = \int_{T_o}^{T} \alpha_L(T')dT'$$

The linear expansion factor (LEF) is another way to look at thermal expansion as a multiplier on the initial length:

$$\mathrm{LEF(T)} = \frac{\mathrm{L}(T)}{L_o} = 1 + \frac{\Delta L}{L} = L_o \left[1 + \int_{T_o}^{T} \alpha_L(T')dT' \right]$$

Correlations to calculate the LEF for several materials are given in Section 3.

When considering changes in volume, the volume coefficient of thermal expansion is defined as:

$$\alpha_V = \frac{1}{V}\frac{dV}{dT}$$

For isotropic materials where expansion occurs evenly in all directions, $\alpha_V = 3\alpha_L$

When calculating thermal expansion, all dimensions increase in size. When evaluating cylinders, both the inner and outer diameters expand outwards. This effect is the same as assuming that the "hole" will expand at the same rate as the material of the cylinder. One way of visualizing the expansion is to imagine that you are resizing a picture. When you make a picture larger, all dimensions increase, even the holes.

In our discussion of thermal expansion, we will assume that the object is not constrained. When the object is constrained, the object may develop *thermal stresses* and not change dimensions as expected.

3. MATERIALS

This section contains the results of a literature search to determine the recommended values of thermal expansion coefficients for common reactor materials.

3.1 Zirconium

The fuel and guide tube claddings are made of zirconium alloys. With thermal expansion, the clad will expand and displace moderator. In addition, the spacer grids are usually composed of zirconium alloys, and zirconium will dictate the thermal expansion of the fuel rod pitch (ppitch).

The TE coefficient for zirconium (and Zirc-2 and Zirc-4) is complicated by two factors. First, there are two phases to the material (an alpha and beta phase). For standard reactor operating conditions, the cladding temperature is less than 1083K, and therefore, the zirconium remains in the alpha phase. The second complication is that zirconium is anisotropic, meaning that the thermal expansion acts differently depending on the orientation of the grain.

For the alpha phase where the crystalline orientation is not known, the recommended diameter and axial TE coefficients are given in [IAEA 2006] in Section 6.2.1.5, page 272.

$$\left(\frac{\Delta L}{L}\right)_{Diam} = -2.128 \times 10^{-3} + 7.092 \times 10^{-6}\, T$$
$$\left(\frac{\Delta L}{L}\right)_{Axial} = -1.623 \times 10^{-3} + 5.458 \times 10^{-6}\, T$$

The original equations assume a base temperature of 300K. However, since the correlations are linear in temperature, an easier way to evaluate them is:

$$\left(\frac{\mathrm{L}}{L_{293}}\right) = 1.0 + \alpha\,(T - T_{293})$$

where $\underline{\alpha_{Diam}=7.092\times10^{-6}\ K^{-1}}$ and $\underline{\alpha_{Axial}=5.458\times10^{-6}\ K^{-1}}$, and the base temperature has been changed from 300K to 293K.

TE coefficients for the beta phase are also given in the IAEA report, but are not needed at standard reactor operating conditions.

The diameter thermal expansion coefficient of α=7.092×10^{-6} K^{-1} agrees reasonably well with other sources, such as Wikipedia, which gives a value of 5.7×10^{-6} K^{-1}. Wikipedia Link

A document from Rice University lists values of 5.7 – 7.0×10^{-6} K^{-1} for pure zirconium, and 5.5-11×10^{-6} K^{-1} for zirconium alloy. Link to Rice University Document

3.2. Stainless Steel

The Watts Bar FSAR states that the bottom nozzle is Type 304 stainless steel and the top nozzle is composed mostly of Type 304L stainless steel. Therefore, this material will dictate the thermal expansion of the assembly pitch as the nozzle expands.

The temperature of the bottom nozzle is approximately equal to the inlet moderator temperature, and the temperature of the bottom nozzle is approximately equal to the outlet moderator temperature. The difference between the inlet and outlet moderator temperatures is only about 20°C, while the change from cold to hot conditions is about 300°C. Therefore, to simplify the models, we can expand both of the nozzles to the average moderator temperature of 310°C (583K). This approximation maintains the same pin pitch axially.

Reference [CINDAS] reports that the material differences between type 304 and 304L are insignificant for thermal expansion. This reference also gives a table of thermal expansion coefficients for SS304 at several different temperatures. The subset of the table over the range 293-1000K is shown below.

Table 3-1: Material Properties for SS304

Temp (K)	Thermal Linear Expansion (%)	Instantaneous Coefficient of Thermal Linear Expansion*	Mean Coefficient of Thermal Linear Expansion*
293	0	14.71	--
300	0.01	14.90	14.78
350	0.086	15.60	15.18
400	0.167	16.27	15.61
500	0.338	17.50	16.33
600	0.519	18.58	16.91
700	0.709	19.49	17.42
800	0.907	20.20	17.89
900	1.112	20.69	18.32
1000	1.323	21.04	18.71

* units 10^{-6} K^{-1}

Interpolating the values at an average moderator temperature of 583K gives a thermal linear expansion fraction of 0.487%, or a LEF of 1.00487. This corresponds to a mean coefficient of linear expansion of α=16.79×10^{-6} K^{-1}.

A second reference gives the TE coefficient for Type 304 SS as 16.9×10^{-6} K^{-1} over the range 0-316°C Balseal Link. This value is very close to the mean coefficient value at 600K given in [CINDAS].

3.3 Pyrex

The TE coefficient for Pyrex is reported as $\alpha=3.25\times10^{-6}\ K^{-1}$ from the Corning property sheet for type 7740 Pyrex at Quartz Link

A graph of the temperature dependence of the TE coefficient of Pyrex is shown in Figure 3.1. This figure shows strong temperature dependence on alpha, but the average value given by the Corning data sheet is reasonable over the temperature range of 20 to 310°C (i.e. CZP to HFP).

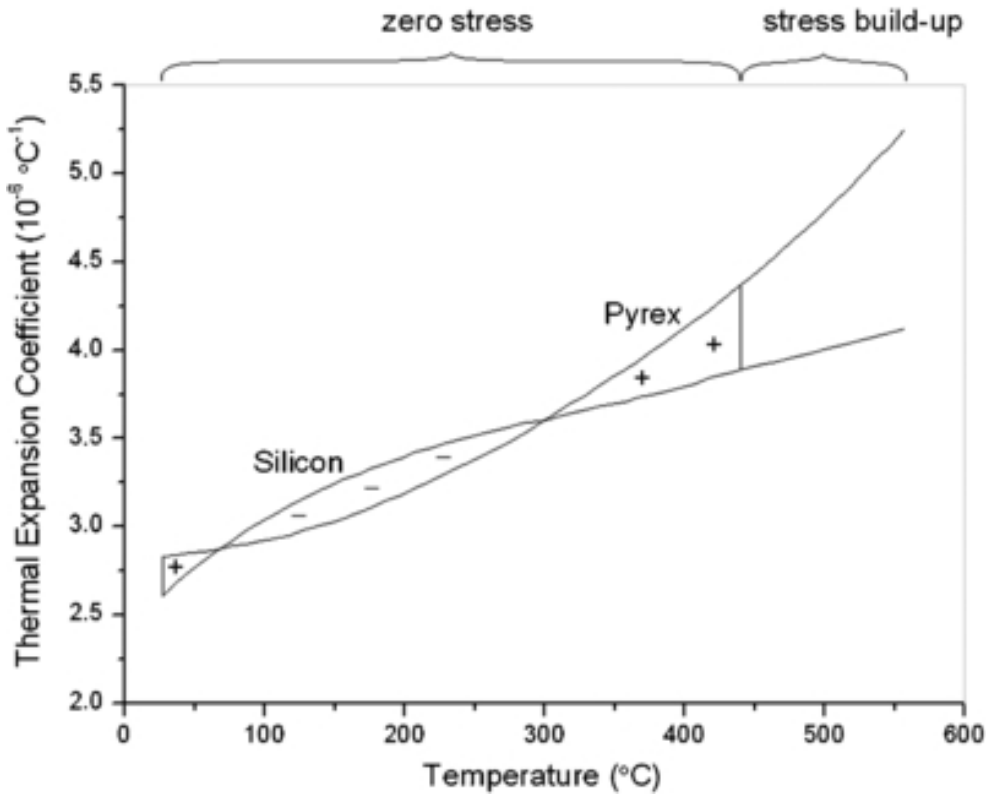

Figure 3.1: Thermal Expansion Coefficient of Pyrex [Mogulkoc Fig. 7]

3.4 Boron Carbide (B_4C)

The TE coefficient for B_4C is given by $\alpha=5.73\times10^{-6}\ K^{-1}$ in [Tsagareishvili].
This value agrees with the range of $5\text{-}6.5\times10^{-6}\ K^{-1}$ given in the online materials database Online Material Database.

The value of $5.73\times10^{-6}\ K^{-1}$ is also reported in [ANT]

3.5 AIC

The TE coefficient for AIC (Ag-In-Cd) is reported as $\alpha=6.9\times10^{-6}\ K^{-1}$ in [ANT], but this value should be confirmed with the values in given in MATPRO. AIC is not a common industrial material and the thermal expansion coefficient is not widely reported.

3.6 Uranium dioxide

The accepted TE coefficient in uranium dioxide is given in [Martin 1988] (and [Fink 2000]).

For fresh UO_2 over the range $273\text{ K} \leq T \leq 923\text{ K}$

$$L = L_{273}(0.99734 + 9.802 \times 10^{-6}\, T - 2.705 \times 10^{-10}\, T^2 + 4.391 \times 10^{-13}\, T^3)$$

and over the range $923\text{ K} \leq T \leq 3120\text{ K}$

$$L = L_{273}(0.99672 + 1.179 \times 10^{-5}\, T - 2.429 \times 10^{-9}\, T^2 + 1.219 \times 10^{-12}\, T^3)$$

One thing to notice is that this equation assumes an initial length specified at 273K, when most of our cold dimensions are specified at 293K. Using the equation above, we can add an additional correction to the length to go from 273K to 293K.

$$L_{273} = L_{293} \times 0.999800$$

The correction introduces an additional multiplication in the above equations.

The UO_2 TE equations are fairly linear over the range 273K to 1200K. If run-time is an issue, we can easily define a single quadratic that would be valid over the entire range 273K to 1500K. The higher order terms only become important as temperatures exceed 2000 K.

The Martin formulas were affirmed in Eq. 7 and 8 of [Fink 2000], and in Section 6.1.1.3 of [IAEA 2006]. The older MATPRO formulation (1979) is NOT recommended, especially at standard operating conditions.

For $(U,Gd)O_2$ fuel, [IAEA 2006] includes a new set of recommendations by Jiang in Section 6.1.3.3 (p. 172). However, the differences between the gad and no gad results are fairly small, and it is therefore not recommended to include a gad dependence on thermal expansion.

3.6.1 Discussion

Martin mentions that the TE data is only valid if "non-reversible shrinkage (sintering) or expansion ("solarization") of samples" has not occurred. Therefore, we must keep in mind that these equations are <u>only valid over a brief interval at BOL</u>. Once the pellets begin to sinter and swell, these equations are no longer valid. In that case, we need to use a fuel performance code to calculate the pellet diameter and density to include the effects of sintering, radiation swelling, creep, etc. versus burnup.

The following figure shows the quantitative behavior of the fuel pellet with exposure (Figure from an INL presentation that credits Dr. Rebecca Weston at BNFL).

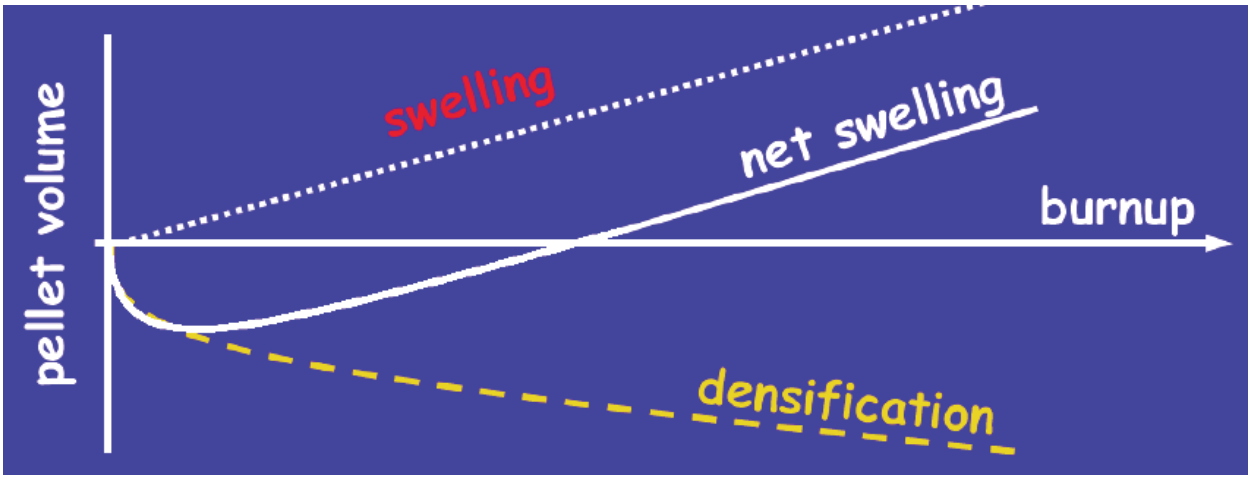

Figure 3.2: Pellet Volume versus burnup

For HZP testing, it is important to use the BOL values. However, as exposure increases, the pellet will sinter, and then swell. Sensitivity studies showing the effects of different pellet dimensions are shown in the results section.

More investigation is needed to quantify the effects of the actual pellet dimensions as a function of burnup.

3.7 Material Summary

Table 3-2: Material Summary

Material	**Thermal Expansion Coefficient (units 10^{-6} K^{-1})**
Zirconium alloys (diameter)	7.092
Zirconium alloys (axial)	5.458
SS304	16.79
Pyrex	3.25
B_4C	5.73
AIC	6.9
Fuel	(use Martin correlation)

TE coefficients for other structural materials need to be determined by the user.

4. EXAMPLE

4.1 Single Assembly Example

This section includes an example of TE in a single assembly problem.

Given the relevant assembly input:

```
mat zirc 6.56 zirc4
apitch 21.50
ppitch 1.26
fuel UO2 10.257 94.5 / 3.1
cell PIN1 0.4096 0.418 0.475 / UO2 he zirc
cell GT          0.561 0.602 /    mod zirc
```

Assume the following temperatures: (taken from a coupled P6 solution)

- average fuel 900 K
- average cladding 610 K
- average moderator 583 K

Look up the corresponding linear expansion factors:

- LEF_fuel 1.006062 from the Martin correlation at the average fuel temperature
- LEF_clad 1.002248 from the IAEA correlation at the average clad temperature
- LEF_ppitch 1.002057 from the IAEA correlation at the average moderator temperature
- LEF_apitch1.004882 from the SS304 table at the average moderator temperature

Note that the LEF for SS304 is more than twice the LEF for zirc.

Radii

The fuel radius increases by the factor LEF_fuel

$$\text{Fuel OR} = 0.4096\ \text{cm} \times 1.006062 = 0.41208\ \text{cm}$$

The inner and outer clad radii increase by the factor LEF_clad

$$\text{Fuel Clad IR} = 0.418\ \text{cm} \times 1.002248 = 0.41894\ \text{cm}$$
$$\text{Fuel Clad OR} = 0.475\ \text{cm} \times 1.002248 = 0.47607\ \text{cm}$$

It should be observed that the gap between the fuel and the clad *decreases* from 0.00840 to 0.00686 cm.

The guide tubes (GTs) also expand, but with the factor LEF_ppitch instead of LEF_clad because the GT cladding is closer to average moderator temperature than the the average fuel clad temperature.

$$\text{GT Clad IR} = 0.561\ \text{cm} \times 1.002057 = 0.56226\ \text{cm}$$
$$\text{GT Clad OR} = 0.602\ \text{cm} \times 1.002057 = 0.60335\ \text{cm}$$

Pin Pitch

The grid dimensions increase by LEF_ppitch, which causes the pin pitch to increase.

$$\text{ppitch} = 1.26\text{ cm} \times 1.002057 = 1.26259\text{ cm}$$

Assembly Pitch

The nozzle dimensions increase by LEF_apitch, which causes the assembly pitch to increase.

$$\text{apitch} = 21.50\text{ cm} \times 1.004882 = 21.60497\text{ cm}$$

The increase in clad OR causes the volume of coolant to *decrease*. However, the increase in assembly pitch causes the volume of coolant to *increase.* The total moderator area increase from the assembly pitch is larger by a factor of almost 5 than the loss of coolant due to clad expansion.

Density

In 2D, the fuel density *decreases* by the factor $(1/\text{LEF_fuel})^2$

$$\text{Fuel density} = \frac{10.257\text{ g/cc}}{(1.006062)^2} = 10.13377\text{ g/cc}$$

In 2D, the fuel clad density *decreases* by the factor $(1/\text{LEF_clad})^2$

$$\text{Clad density} = \frac{6.56\text{ g/cc}}{(1.002248)^2} = 6.53060\text{ g/cc}$$

The guide tube clad density *decreases* by the factor $(1/\text{LEF_ppitch})^2$. This example demonstrates a case where a single material density needs to be adjusted at two different temperatures.

In 3D calculations, the density decreases by another factor to account for axial expansion. However, the axial factor depends on how the 3rd dimension is expanded. If all all of the materials are expanded in the axial direction by a common factor (e.g. the fuel LEF), then all of the densities must decrease by same factor (1/LEF_fuel). The factor used to decrease the densities for axial expansion must be consistent with the dimensional change to preserve total mass.

Final Results

After the thermal expansion of the fuel, clad, and pitch have been accounted for, the new input becomes:

```
mat zirc 6.53060  zirc4
apitch 21.60497
ppitch 1.26615
fuel UO2 10.13377 94.5 / 3.1
cell PIN1 0.41208 0.41894 0.47607 / UO2 he zirc
cell GT           0.56226 0.60335 /    mod zirc
```

In this example, the zirconium density has been adjusted with the average clad temperature. In the MPACT implementation, there needs to be two density corrections, one for the fuel clad temperature and one for the guide tube temperature.

Note that the second density in the "fuel" card has not been adjusted. This value is intended to be used to look up fuel material properties in fuel performance calculations, and is not currently being used in the codes.

4.2 Axial Expansion

Expanding the geometry in the axial direction introduces several issues. If each material (zircaloy, fuel, absorber material) is allowed to expand independently, then most of the existing axial levels will need to be modified by the code. For example, if the fuel expands axially at a rate greater than the clad, then the upper plenum region will need to be adjusted to make the plenum smaller. This adds a lot of complexity to the code logic, and possibly additional axial planes to the geometry.

Fortunately, the effects of axial expansion are smaller than the effects of radial expansion and a simplified axial expansion model can be implemented that assumes that all materials expand in the axial direction at the same rate. Assuming the fuel is the most important material in the core, it makes sense to expand all materials with the fuel LEF in the axial direction.

If a simplified axial expansion is used, the following geometries must all be expanded using the same axial factor:

- total height
- assembly axial levels
- assembly grid heights
- assembly grid locations
- assembly upper and lower nozzle heights
- edit boundaries

All of the material densities used in the core must be decreased by the same axial factor (1/LEF) so that the total mass of the materials is conserved. For example, the clad density would be decreased by $1/(LEF_{clad}^2\ LEF_{fuel})$ since the clad material is expanded in the radial direction by the clad thermal expansion coefficient, and in the axial direction by the fuel thermal expansion coefficient.

The upper and lower core plates must also be expanded, but these can be expanded with the actual core plate materials because they do not "share" an axial level with any other geometry object.

4.3 Absorber Materials

The 2D example in Section 4.1 did not include any materials inserted into the guide tubes (control rods, WABA, Pyrex, detectors, etc.) These objects must be thermally expanded at the average moderator temperature.

5. RESULTS

To determine the effects of thermal expansion, a small utility program has been written which modifies the XML file to expand all of the dimensions, and adjust the densities.

Since the TE adjustments are made at the XML level, a small approximation is made that each material is only adjusted at a single temperature. This approximation will not be necessary to make in the MPACT implementation.

5.1 Pincells (BOL)

The first set of results is to the 360 pincells problems from [CASL-1] run with and without TE. The expanded dimensions include the fuel pellet, clad, and pin pitch. Since these are pincell problems, the pin pitch was adjusted as an assembly pitch (i.e. expand nozzle instead of spacer grids) to capture the total change in moderator volume.

As expected, the boron concentration has a large impact on the TE results. This effect is due to the increase in coolant as the pin pitch increases. If the moderator includes a lot of boron, the total absorptions will increase and decrease the eigenvalue. As the boron concentration decreases, this additional absorption is decreased. Therefore, adding TE to MPACT will add a trend in the BOL-EOL boron results for full core problems as the boron concentration decreases through the cycle. The TE effect is 200 pcm over the range of boron typically found in a reactor cycle.

The pin enrichment has a larger than expected impact on TE. This effect is assumed to be due to the decrease in resonance escape as the pin diameter increases, and the enrichment has a large effect on the resonance escape. This effect is harder to model because we do not have a good model of the actual fuel pellet diameter as a function of burnup in MPACT. See Section 5.4 for more discussion.

The fuel type, moderator density, and fuel temperature do not have a large impact on the TE effects.

The following tables shows the change in eigenvalue with thermal expansion versus no thermal expansion. The first row is the average over all 324 hot cases. The remaining rows are averages over specific parameters so we can evaluate trends versus parameter. For example, TE will increase the eigenvalue 193 pcm with there is no boron, but will decrease the eigenvalue 8.1 pcm when there is 1300 pcm boron.

Table 5-1: Pincell Differences with Thermal Expansion (pcm)

		Ave	Sdev	Min	Max	Count
All hot	All	90.9	96.3	-139.2	278.9	324
Type	beav	51.5	97.0	-139.2	226.7	81
Type	krsko	124.2	89.8	-56.7	278.9	81
Type	surry	90.8	93.1	-91.3	245.7	81
Type	wb	97.1	92.5	-85.3	257.0	81
Enrich	21	41.5	97.5	-139.2	217.9	108
Enrich	31	98.0	88.5	-74.6	258.8	108
Enrich	41	133.1	79.7	-27.6	278.9	108
Boron	0	193.4	39.8	86.0	278.9	108
Boron	600	87.3	51.3	-39.4	193.6	108
Boron	1300	-8.1	57.2	-139.2	109.4	108
Density	den1	73.4	98.7	-139.2	256.1	108
Density	den2	89.4	95.8	-120.3	266.3	108
Density	den3	109.9	91.7	-95.3	278.9	108
Tfuel	600	100.7	99.6	-124.9	278.9	108
Tfuel	900	90.3	95.8	-131.5	259.7	108
Tfuel	1200	81.6	93.4	-139.2	247.4	108

* results = (thermal expansion) – (no thermal expansion)

A typical worth of boron in a PWR is 8 pcm/ppm. Therefore a 200 pcm change in eigenvalue is approximately equal to 25 ppm boron.

5.2 2D Assemblies (BOL)

The next set of results is the VERA2 assembly geometry with the extended set of 90 statepoints from [CASL-2]. These cases were run with and without TE to confirm that the pincell sensitivities also apply to single assemblies. The difference between the eigenvalues is shown in Table 5-2. (Only 81 results are included because nine of the assemblies are at cold conditions and do not have any thermal expansion.)

The assembly cases show the same trends as the pincell cases. Boron and enrichment have a larger impact on the thermal expansion effects. The moderator density and fuel temperatures have a smaller impact.

Table 5-2: Assembly Eigenvalue Differences with Thermal Expansion (pcm)

		Ave	Sdev	Min	Max	Count
Type	wb2a	52.2	93.4	-129.9	213.9	81
Enrich	21	2.4	94.1	-129.9	144.6	27
Enrich	31	58.8	86.1	-66.1	189.1	27
Enrich	41	95.2	77.8	-20.2	213.9	27
Boron	0	155.7	34.1	88.6	213.9	27
Boron	600	47.5	44.5	-33.0	119.5	27
Boron	1300	-46.7	49.0	-129.9	30.6	27
Density	den1	36.9	96.9	-129.9	193.2	27
Density	den2	50.9	94.0	-112.7	202.5	27
Density	den3	68.7	90.0	-90.5	213.9	27
Tfuel	600	61.6	98.1	-120.9	213.9	27
Tfuel	900	55.2	94.5	-122.0	201.5	27
Tfuel	1200	39.7	89.7	-129.9	178.2	27

* results = (thermal expansion) – (no thermal expansion)

In addition to the eigenvalue results, the change in pin power was also examined for all of the assembly cases. The results are shown in the next table.

Table 5-3: Assembly Pin Power Differences with Thermal Expansion

	Ave (%)	Min (%)	Max (%)	Count
Maximum pin power difference in assembly	2.24	2.69	1.79	81
RMS Difference in assembly	0.70	0.82	0.57	81

All of the maximum pin power differences occurred in the corner fuel pin. The corner fuel pin is affected the most because the assembly gap increases with thermal expansion, and the corner fuel pin will see a larger increase in moderator volume. Using the values from Section 4, the assembly gap will increase from 0.08 cm to 0.141 cm.

5.3 Sensititivies (BOL)

In this section, a subset of the 2D assembly cases is run to determine the sensitivity of local temperatures (and/or linear expansion coefficients) used in the thermal expansions. The question that these cases are trying to answer is "how sensitive are the results to local temperature changes and/or the value of the linear expansion coefficients?"

For each case, the temperature used to perform the TE (fuel, clad, moderator) is perturbed to cover the range of temperatures actually encountered in a reactor. The temperature changes are repeated for three assemblies used in Section 5.2 that had a low, nominal, and high TE effect.

- The low TE assembly is "wb2a-21-1300-den1-1200", that had a -129.9 pcm change from TE
- The nominal TE assembly is "wb2a-31-0600-den2-0900" that had a +56.5 pcm change from TE
- The high TE assembly is "wb2a-41-0000-den3-0600", that had a +213.9 pcm change from TE

The eigenvalue results are shown in Table 5-4. The results are relative to the TE cases with the "standard" temperature.

Table 5-4: Eigenvalue Results of Temperature Perturbations (pcm)

CASE	Expansion Temp (K)	Low Assembly	Nominal Assembly	High Assembly
Clad A	300	-22.1	19.8	53.9
Clad B	580	-2.1	1.8	5.0
Clad C	610	--	--	--
Clad D	640	2.2	-1.8	-5.1
Mod A	300	117.3	-105.4	-281.5
Mod B	566	10.2	-8.0	-15.1
Mod C	583	--	--	--
Mod D	602	-6.9	6.2	23.7
Fuel A	300	24.8	34.9	44.3
Fuel B	600	8.3	12.4	16.5
Fuel C	900	--	--	--
Fuel D	1200	-12.7	-18.4	-23.7
Fuel E	nogap	159.9	-90.9	-174.9

The set of rows labeled "Clad" show the results of expanding the fuel cladding at different temperatures. Going from cold conditions to nominal (610K) show a relatively large change (Row A), and changes +/- 30K around nominal show a smaller eigenvalue change (Rows B and C). These results show that the using the exact local clad temperature is not as important as going from cold to hot. This result leads us to the conclusion that <u>we can expand all clad dimensions at the same average clad temperature for the entire core</u>.

The set of rows labeled "Mod" show the results of expanding the pin pitch and GT materials at different temperatures. Going from cold conditions to nominal (583K) show a relatively large change (Row A), and changes about +/- 20K around nominal show a smaller change (Rows B and C). These results show that using the exact local moderator temperature is not as important as

capturing the large change from cold to hot. This result leads us to the conclusion that we can expand the pin pitch and GT materials at the same average moderator temperature for the entire core.

The set of rows labeled "Fuel" show the same basic trends as the clad and pitch, except that the local changes are more significant when compared to the change from cold to hot. This comparison is somewhat troubling because it may indicate that we need to expand the fuel pellet at the local fuel temperature, not some average fuel temperature. In fact, we know that the fuel rod keeps expanding until the gap eventually closes. Row "Fuel E" shows the eigenvalue change in removing the gap completely (expanding the fuel pellet diameter to the clad inner radius). This is an extreme cast that is unphysical, but it does show that the effect of removing the gap completely can be larger than the total effect of thermal expansion.

In conclusion:

- we can expand all of the fuel clad in the core to the average clad temperature
- we can expand all of the pin pitches and GT materials in the core to the average moderator temperature
- we may have to account for the local fuel temperature expansion, especially as the gap closes

5.4 2D Assemblies (Depletion)

The same three assemblies as used in the last section (low, average, and high assemblies) are depleted to examine the effects of TE change with depletion.

In the previous section, it was shown that the results are fairly insensitive to the cladding and moderator temperatures used in the TE; however there is a somewhat significant dependence on the fuel temperature used in the TE. To investigate the fuel temperature dependence further, the following graphs show the results of expanding the fuel pellet at four different temperatures to get an idea of the sensitivity of the fuel temperatures used in the expansions. (The actual fuel temperature was not changed, only the temperature used in the thermal expansion of the fuel pellet.) In addition, a rather extreme case was run where the gap is completely closed (the fuel pellet was expanded to touch the inner clad radius). This total gap closure is not physical, but it does provide an upper bound on the sensitivities.

The dashed line shows the "best estimate" curve where the pellet gap starts open, and then expands linearly until the gap is closed at 15 GWd/MT. This curve assumes the gap will close at the end of the first cycle, which is approximately 15 GWd/MT.

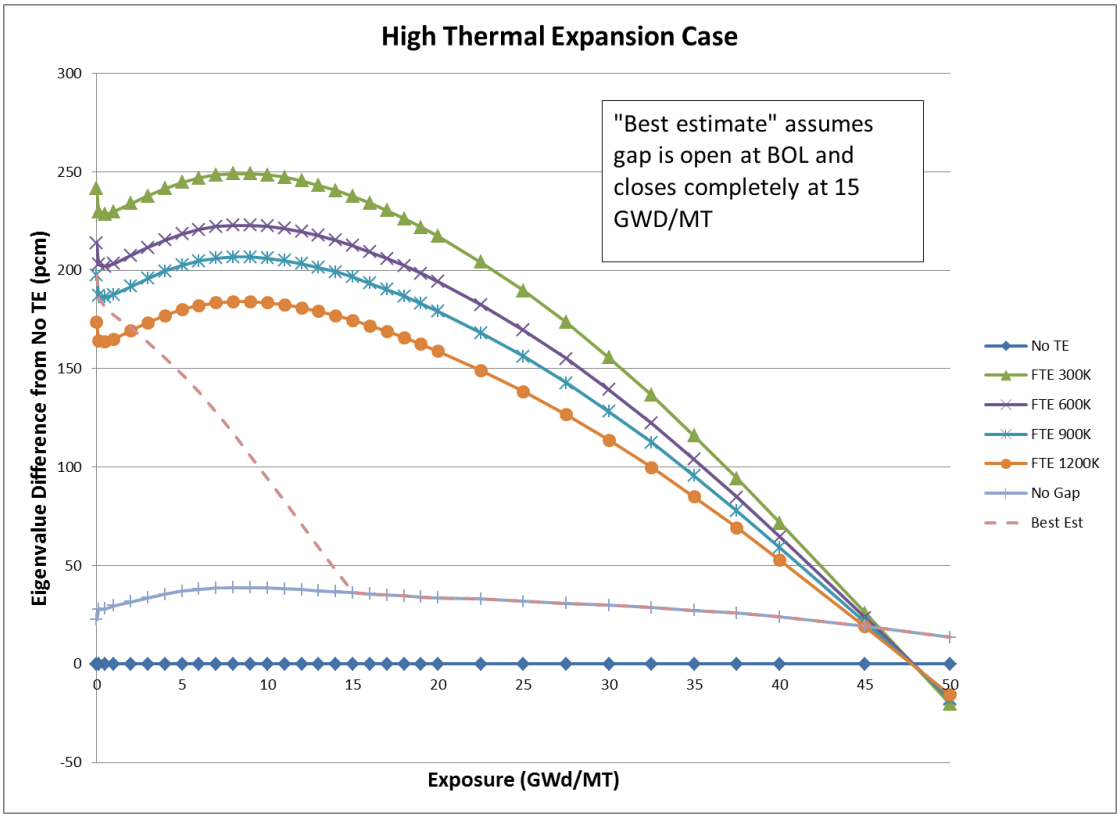

Figure 5.1: High thermal expansion results vs. depletion

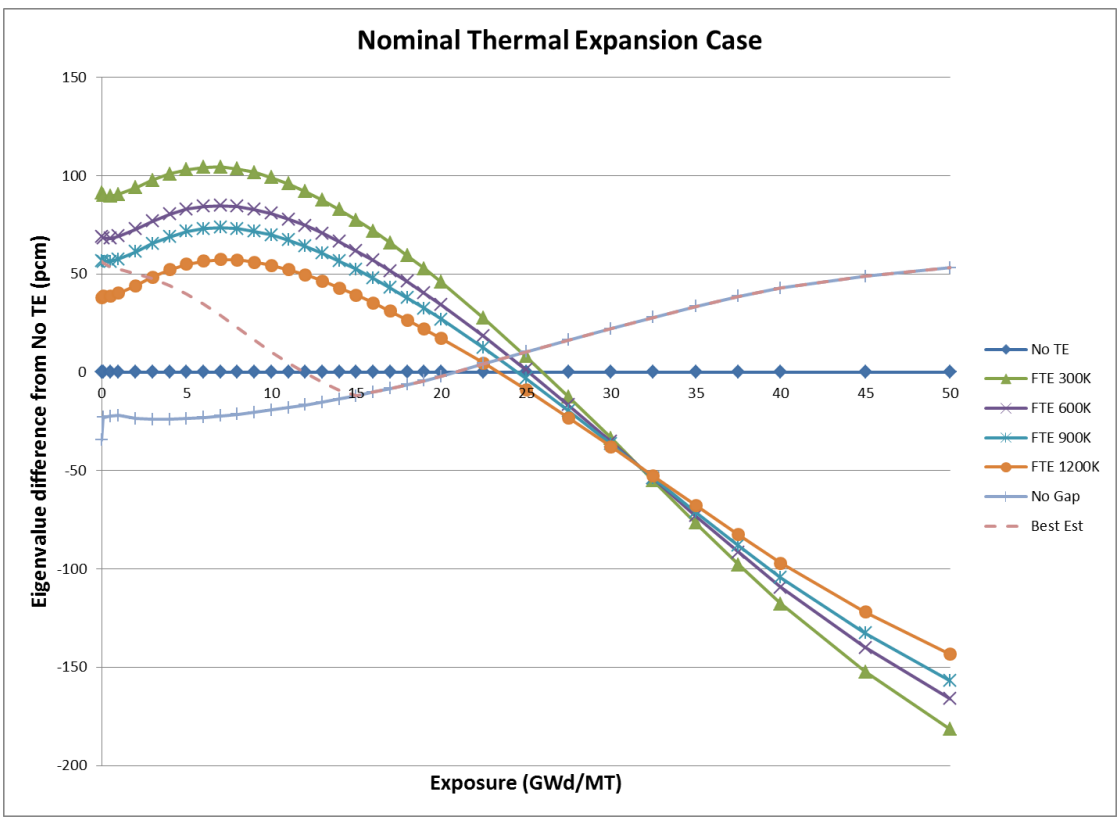

Figure 5.2: Nominal thermal expansion results vs. depletion

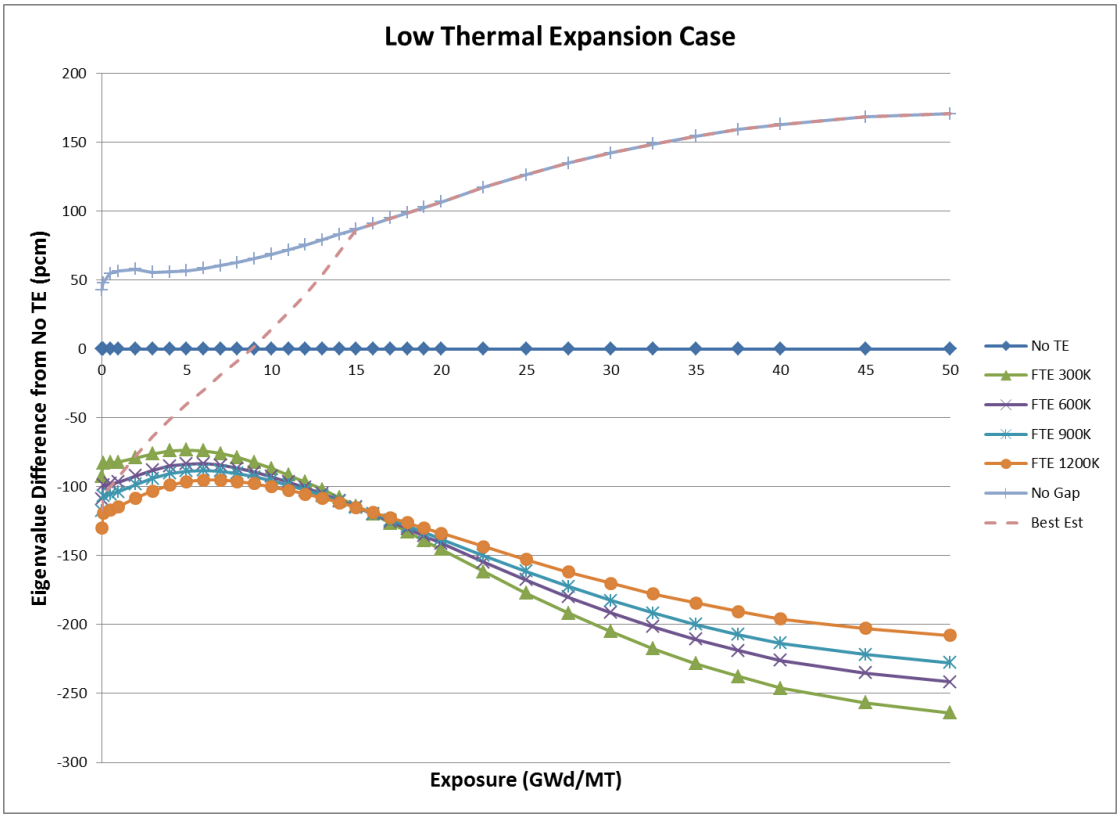

Figure 5.3: Low thermal expansion results vs. depletion

All of the assemblies are run with a constant boron concentration. During core calculations, there will be an additional effect as the boron concentration decreases during the cycle.

In conclusion:

- The effect of TE with exposure is somewhat large (~200 pcm over the life of the fuel) due to the history effects introduced by a geometry change.
- There are additional TE effects due to the boron concentration that are not captured in these graphs.
- The uncertainty in the temperature used to expand the fuel pellet introduces an uncertainty into the TE results. This uncertainty can be +/- 50 pcm.
- There is an additional uncertainty due to pellet densification and swelling. This uncertainty may be on the same order, or larger, than the temperature uncertainty.
- We need to investigate the effects of fuel pellet size versus burnup further. Several suggestions are presented in Section 6.

5.5 3D Assemblies

Progression Problem 6 (single assembly with feedback) was run with and without TE turned on. This problem includes both thermal expansion effects and thermal-hydraulic feedback effects.

The results are shown in Table 5-6. Results are shown using both 2D thermal expansion (only expansion in the radial direction) and 3D thermal expansion (expand in both the radial and axial directions). The results are repeated for three different boron concentrations – 0, 600, and 1300 ppm.

Table 5-6: Thermal Expansion Results for 3D Assembly

Expansion Method	Boron (ppm)	Eigenvalue Diff (pcm)	Max Pin Diff (%)	RMS Pin Diff (%)	Diff Max Pin (%)
2D	0	180.6	3.66	0.87	-0.78
2D	600	73.1	3.48	0.87	-0.77
2D	1300	-23.2	3.53	0.88	-0.52
3D	0	255.5	3.70	0.88	-0.76
3D	600	100.7	3.54	0.93	-0.81
3D	1300	-37.9	3.69	1.02	-0.51

The Problem 6 results confirm the pincell and single assembly results, which showed an approximate +200 pcm increase in eigenvalue when going from 1300 to 0 ppm boron. The maximum change in pin power is approximately 3.5%, and the largest change always occurs in the corner rod.

The 3D results also show that there is not much difference between using the 2D TE models (radial only) and 3D TE models (radial and axial). This result is expected since the main effects of TE are to increase the moderator volume and fuel pellet diameter in the radial direction.

Since it is fairly easy to implement a simplified axial expansion model, it is recommended that we implement 3D TE in MPACT.

5.6 2D Assemblies (ITC)

One question that keeps coming up is the effect of TE on the isothermal temperature coefficient (ITC). To answer this, three 2D assemblies were run using the VERA2A assembly geometry and ITC conditions. These cases were run with:

- A base case at 557 °F and moderator density 0.75133 g/cc
- A perturbed case at 662 °F and moderator density 0.74549 g/cc
- BOL conditions with 1300 ppm boron
- With and without thermal expansion (TE)
- Three different U-235 enrichments (2.1, 3.1, and 4.1%)

The results and corresponding ITC values are shown in Table 5-7.

Table 5-7: ITC Results

	U-235 enrichment	Eigenvalue T=557°F	Eigenvalue T=562°F	ITC	
no TE	2.1	1.05451	1.05516	12.37	pcm/°F
no TE	3.1	1.18175	1.18203	4.72	pcm/°F
no TE	4.1	1.26070	1.26070	0.05	pcm/°F
TE	2.1	1.05325	1.05393	12.92	pcm/°F
TE	3.1	1.18115	1.18145	5.21	pcm/°F
TE	4.1	1.26057	1.26060	0.50	pcm/°F

One conclusion is that the ITC has a very strong dependence on enrichment.

The second conclusion is that TE tends to *increase* ITC by about 0.5 pcm/°F for all enrichments. Modeling TE should help improve our full-core simulator ITC results, which tend to be *low* by about 0.8 pcm/F.

6. IMPLEMENTATION REQUIREMENTS

The following is a list of implementation requirements. There are several "suggested features" that are optional and not required.

These requirements should be implemented into MPACT as soon as possible. It is also recommended that additional studies be performed to determine the actual gap closure behavior versus burnup, and possibly implement additional models to account for the actual pellet diameter.

Input

1. There should be a single on/off switch to turn TE on and off. This switch will help us perform TE sensitivity studies and also allow code-to-code comparisons with codes that do not have thermal expansion.
2. Each material (except fuel) should have a TE coefficient in the input. These values should be added to the default material definitions (i.e. added to the INI files). Fuel materials should use the TE correlation from [Martin 1988]. The preferred units of the TE coefficients are "10^{-6} K^{-1}"
3. Sanity checks should be made to make sure that the TE coefficients have been entered by the user and are "reasonable" values.
4. There should be a user input for average temperature values of the moderator, cladding, and fuel. (These values can be obtained by first running a coupled calculation without TE and looking at the edits of the average clad, moderator, and fuel temperatures). These temperatures should only be used for TE. The preferred units are "K".
5. For cases with feedback (either CTF or internal T/H models), an option should be added to calculate the average moderator temperature using a global energy balance:

   $$Q = \dot{m} C_p \Delta T$$

   The internal T/H steam tables can be used for this calculation, even if CTF coupling is enabled. The calculated value should be printed to the output.
   If this option is used to calculate the average moderator temperature, the average clad temperature should be calculated as

   $$T_{cladave} = T_{modave} + 30\ K * \frac{\%power}{100\%}$$

   The average fuel temperature should be calculated as:

   $$T_{fuelave} = T_{modave} + 320\ K * \frac{\%power}{100\%}$$

   The factors of "30K" and "320K" should be user input values with defaults.
6. [Suggested feature] The code should have a special input flag to eliminate the fuel gap by <u>expanding the fuel pellet</u> out to the clad inner radius. This option should be available with and without TE to perform sensitivity studies (The code should track this flag on an assembly-by-assembly basis).
7. [Suggested feature] The code should have a special input flag to eliminate the fuel gap by <u>shrinking the clad material</u> to the fuel pellet radius. This option should be available with and

without TE to perform sensitivity studies (The code should track this flag on an assembly-by-assembly basis).

8. [Suggested feature] When performing a core shuffle, there should be a flag to eliminate the gap on all burned fuel read from a restart file (i.e. not fresh fuel). This flag should only be available in a core shuffle case. This feature is used to simulate the gap closing at approximately the end of the first cycle.

Radial Expansion

The following geometry object dimensions should be thermally expanded in the radial direction and the corresponding material densities adjusted.

1. The pin pitch (ppitch) should be thermally expanded using the input average moderator temperature and the TE coefficients for the dominant spacer grid materials. The pin pitch dimensions should increase as discussed in the Section 4. If the spacer grids have different materials, the average coefficient should be used to expand "ppitch". The spacer grid material density does not need to be adjusted since it is smeared in the water.
2. The assembly pitch (apitch) should be expanded using the input average moderator temperature and the TE coefficient for the core plate materials (i.e. do not include smeared water). The assembly pitch dimensions should increase as discussed in Section 4. The core plate material density should be reduced for the 2D radial expansion. If the top and bottom core plates have different materials, the average coefficient should be used to expand "apitch" and adjust the material densities.
3. Since we do not know the width of the top and bottom nozzles, the nozzle density should be reduced for the 2D radial expansion using the LEF of the core plates.
4. All radii in the "cell" cards should be expanded using the corresponding material TE coefficients and the following temperatures: fuel material should be expanded using the average fuel temperature, fuel cladding materials should be expanded using the average clad temperature, and all guide tube materials and inserts should be expanded using the average moderator temperature. The corresponding material densities should be reduced for the 2D radial expansion using the corresponding material TE coefficients. All radial dimensions should increase and the material densities should decrease.
5. If one of the special input flag is set, the fuel pellet radii should be expanded to the same size as the clad inner radii (after clad has been expanded), or the clad should be shrunk down to the pellet size. The fuel density should be decreased accordingly. This option should be available for either all assemblies, or just the assemblies that are read from a restart file. (Another way to implement this flag is to close the gap on any assembly that has a burnup greater than some small value like 1.0 GWd/MT.)

Axial Expansion

1. The following geometry objects should be thermally expanded using the average fuel temperature and the fuel expansion coefficient given by [Martin]:
    - total height
    - assembly axial levels
    - assembly grid heights
    - assembly grid locations
    - assembly upper and lower nozzle heights
2. All of the densities listed in the section on "Radial Expansion" should also be decreased by the fuel LEF to account for the thermal axial expansion. (The density will be decreased by the material LEF for 2 radial directions, and for the fuel LEF in the axial direction).

CTF

1. The TE of the pitch (apitch and ppitch) and cladding need to be added to the CTF preprocessor. The CTF calculation can ignore the fuel pellet expansion if fuel temperature tables are used. The CTF calculation can also ignore any changes to material density.

Issues

1. The same material may be used in multiple places with different temperatures (e.g. clad material may be used in fuel rods and in burnable absorber rods). Therefore, the density expansion should happen when the material is used, not at the beginning of the calculation.
2. It is suggested that the "LEF" be stored for each geometric object and applied when number densities are calculated. Both dimensions and materials must be expanded.
3. One potential error could occur if users have "stacked cases" where the power is changing during runs. If the thermal expansion is only done once, then the thermal expansion will be done at the temperature of the first case. If the user had a stacked HZP and HFP case, the HFP thermal expansion would be wrong. This won't be an issue for small power changes, but it may have an effect from HZP to HFP.

7. CONCLUSIONS

This report investigated the effects of modeling thermal expansion in MPACT.

The results show that the main effect of adding thermal expansion is the increase in the moderator flow area in the radial direction. The effects of the increased moderator flow area decrease the eigenvalue at BOC conditions (with high boron concentrations) and increase the eigenvalue at EOC conditions (with lower boron concentrations). The boron effect could have a small improvement on our boron letdown curves when compared to measured data.

Another positive effect of adding thermal expansion is an increase in our calculated ITC results of 0.5 pcm/^{o}F. Our current ITC results are low by approximately 0.8 pcm/^{o}F, so adding TE models should improve our comparisons of calculated ITC with measured data.

An unexpected result of adding thermal expansion models to MPACT is a fairly high sensitivity to the fuel pellet dimensions and U-235 enrichment. This sensitivity is due to the change in the resonance escape probability and thermal utilization. It is recommended that further studies be performed to determine the actual pellet dimensions as a function of burnup (including thermal expansion, sintering, and swelling), and to evaluate the effects of changes of the pellet size on the neutronics calculations.

It was shown that most of the thermal expansion effects can be captured by expanding the reactor dimensions in the radial direction only. These results are consistent with the largest effects being from the increase in moderator flow area and change in pellet diameter. However, since it is fairly straight-forward to expand the dimensions in the axial directions as well as the radial directions, it is recommended that we implement 3D expansion in MPACT.

Finally, a set of implementation requirements was developed for adding thermal expansion models to MPACT.

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