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Modeling Thermal Expansion in VERA-CS

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Abstract - *This paper describes the implementation of modeling thermal expansion in the CASL core simulator code VERA-CS. The effects of thermal expansion are first investigated and quantified using single-pin and single-assembly models, and then the effects on full-core calculations are described. This paper shows that the effect of thermal expansion on core-follow critical boron calculations is fairly small (approximately 10 ppm boron), but the effects on ITC and power defect can be significant.*

I. INTRODUCTION

The Consortium for Advanced Simulation of LWRs (CASL) has developed a high-fidelity core simulator, named VERA-CS, for modeling commercial pressurized water reactors (PWRs) [1]. This paper describes the implementation of modeling thermal expansion (TE) in VERA-CS. This represents the first implementation of thermal expansion in a high fidelity simulator that does not rely on pre-generation of cross sections or significant homogenization of the geometry.

Thermal expansion of materials is an important effect to model in reactor physics. Geometric design information in reactor documentation is usually given at room temperature (cold conditions), but the core is operated at much higher temperatures (hot conditions). The typical inlet temperature of PWRs is around 300 C. All components in the reactor vessel thermally expand due to this temperature change. The core plate expands radially, altering the assembly pitch. The grid spacers in an assembly expand changing the pin pitch within the lattice. The fuel and control rods expand axially. The fuel pellet and fuel rod cladding also expand radially. These effects in combination on are neutronically important and modeling the effects of TE have existed in the standard industry tools for a number of years. Reference [2] asserts that in order to achieve an accurate high fidelity simulation capability, thermal expansion should modeled.

In current industry practice, few-group cross sections are pre-calculated with a lattice physics code run at specified temperatures. The few-group cross sections are then tabulated in a look-up table as a function of temperature (and other parameters) to be used by the core simulator. Since the fuel and moderator temperatures are specified in the lattice physics input, the TE is fairly easy to implement and few-group cross sections automatically have TE included.

In VERA-CS, the whole core is modeled using reactor physics methods typically found in lattice physics codes, except that the local temperatures are determined from thermal-hydraulic feedback. As such, the local temperatures are not known *a priori*, are not usually uniform, and evolve during the solution process. If TE was modeled using the local temperatures, the geometry processing would have to be repeated at each iteration. However, as will be shown in this paper, most of the thermal expansion effects are adequately captured by expanding the materials from cold conditions to the average hot conditions, while ignoring the differences between the local local temperatures and average hot temperature. As such, VERA-CS performs thermal expansion by expanding all the geometry at average hot conditions before starting the calculation.

The theory of thermal expansion is developed and briefly summarized in the following section. Following this, a review of the literature and recommendations for thermal expansion coefficients are given. Next, the implementation of thermal expansion in VERA-CS is described. Finally, results of thermally expanded calculations are presented that quantify the effects of the thermal expansion on reactivity and power distribution for several models.

II. THEORY

For solid materials with an isotropic crystal structure, the equation for the change in dimension in any direction due to linear thermal expansion of the material is given by:

$$\Delta L = \alpha_L \, L_0 \, \Delta T \tag{1}$$

where α_L is is the coefficient of linear thermal expansion, L_0 is the initial length (at some reference temperature), and ΔT is the change in temperature from the reference temperature.

For cases where α_L is a function of temperature, it is often easier to consider the total change in linear dimension

$$\frac{\Delta L}{L_0} = \int_{T_0}^{T} \alpha_L(T') \, dT' \tag{2}$$

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

$$\mathrm{LEF}(T) = \frac{L(t)}{L_0} = L_0 \left[1 + \int_{T_0}^{T} \alpha_L(T') \, dT' \right] \tag{3}$$

Correlations to calculate the LEF for several materials are given in the next section.

To preserve mass when thermally expanding the geometry, the material densities need to be modified to be consistent with the expanded dimensions. The density is modified according to:

$$\rho(T) = \rho_0 \, \frac{V_0}{V(T)} = \rho_0 \left(\frac{L_0}{L(T)} \right)^3 = \frac{\rho_0}{LEF(T)^3}. \tag{4}$$

III. REACTOR MATERIAL PROPERTIES

The main components of thermal expansion in a reactor consist of just a few materials. In this section we present the correlations used to obtain the thermal expansion coefficients for each of those materials.

Zirconium Alloys

Fuel and guide tube cladding is usually composed of zirconium alloys (either Zircaloy-2 or Zircaloy-4) in light water reactors. With thermal expansion, the clad will expand and displace moderator. In addition, the spacer grids are usually composed of zirconium alloys, and zirconium will also dictate the thermal expansion of the fuel rod pitch.

The TE coefficient for zirconium (and Zircaloy-2 and Zircaloy-4) is complicated by two factors. First, there are two phases to the material (an α- and β-phase). For standard reactor operating conditions, the cladding temperature is less than 1083 K, and therefore, the zirconium remains in the α-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 α-phase where the crystalline orientation is not known, the recommended diameter and axial TE coefficients are given in [3]. These equations are:

$$\left(\frac{\Delta L}{L}\right)_{\text{radial}} = -2.128 \times 10^{-3} + 7.092 \times 10^{-6}\, T \qquad (5)$$

$$\left(\frac{\Delta L}{L}\right)_{\text{axial}} = -1.623 \times 10^{-3} + 5.458 \times 10^{-6}\, T \qquad (6)$$

These equations have been implemented in VERA-CS for all zirconium alloys. Note that the zirconium equations shown are based on a reference temperature of 300 K. The equations are adjusted internally in VERA-CS to convert to the standard reference temperature of 293 K.

Stainless Steel

The reactor core plate is composed stainless steel. Additionally, it is not uncommon to have nozzles that are made of stainless steel. The most common types of stainless steel used inside reactor vessels are types 304 and 304L. According to [4], the material differences between 304 and 304L are insignificant for thermal expansion. This reference also gives a table of thermal expansion coefficients for SS304 for temperatures ranging from 10 K to 1600 K which adequately covers reactor operating temperatures. Interpolation of this table is used to obtain the thermal expansion coefficient of stainless steel.

Uranium Dioxide

The accepted TE coefficient for uranium dioxide is given in [5] and [6]. This correlation applies only to fresh UO_2 fuel. Once the pellet begins to sinter and swell, other physics become important to predicting the dimensional changes of the pellets. The models suggested by [6] are used to determine the thermal expansion coefficients of the fuel. Additional work is on-going to use a fuel performance code to determine the dimensions of the fuel pellet with additional physics.

Pyrex

The TE coefficient for Pyrex is reported as 3.25×10^{-6} K^{-1} from the Corning property sheet for type 7740 Pyrex [7]. Reference [8] shows the temperature dependence of the TE coefficient of Pyrex varies by approximately 0.6×10^{-6} K^{-1} compared to the value reported in [8]. Therefore, the constant value of 3.25×10^{-6} K^{-1} is used in VERA-CS.

Boron Carbide

The TE coefficient for boron carbide (B_4C) is reported as 5.73×10^{-6} K^{-1} in [9].

Silver-Indium-Cadmium

The TE coefficient for AIC (Ag-In-Cd) is reported as $6.9{\times}10^{-6}$ K^{-1} in [10]. AIC is not a common industrial material and the thermal expansion coefficient is not widely reported in the literature.

Material Summary

A summary of the thermal expansion coefficients for common reactor materials is shown in Table I. The largest dimensional changes occur in stainless steel.

TABLE I. Summary of typical thermal expansion coefficients.

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)

IV. IMPLEMENTATION

The implementation of thermal expansion in VERA-CS is performed through an input preprocessor. VERA-CS uses a common input deck to feed all of the coupled multiphysics codes. In this sytem, an XML input file is generated from the VERAIn [11] ASCII input processor. The thermal expansion is implemented by processing the XML file and adjusting the core dimensions for thermal expansion. This approach is needed since VERA-CS consists of several codes (transport, thermal hydraulics, Monte Carlo, fuel performance, etc.), each with their own mesh and model construction. This solution allows a single thermal expansion model to work with many different physics codes instead of having each physics code multiple thermal expansion implementations.

The preprocessor uses user-specified expansion temper-

atures (usually core average) and the previously reported expansion coefficients for the various reactor components. Users may also provide their own thermal expansion coefficients for additional materials defined in the model.

V. RESULTS

To quantify the effect of TE, several models are evaluated. First a suite of pincells developed for verification of VERA-CS [12] are evaluated for trends. Then a suite of lattices [13] are evaluated. For a few prototypical lattices, the sensitivity to local TE effects are quantified. Lastly, 3D core results are presented for a typical cycle depletion, power defect cases, isothermal temperature coefficient cases, and a baffle sensitivity study.

1. Pincells (BOL)

The first set of results is the test suite of pincell problems from [12] run with and without TE. The pincell test suite includes

- four pincell geometries (BEAVRS, Krško , Surry, and Watts Bar),
- three fuel enrichments (2.1, 3.1, and 4.1% U-235),
- three boron concentrations (0, 600, and 1300 ppm),
- three moderator densities (inlet, average, and outlet), and
- three fuel temperatures (600, 900, and 1200 K),

for a total of 324 hot cases. There are additional pincell cases specified in the test suite at cold conditions, but these are not relevant for thermal expansion studies.

The temperatures used for the thermal expansion cases were 583 K for the moderator, 610 K for the cladding, and 900 K for the fuel. The expanded dimensions include the fuel pellet, cladding, and pin pitch. The pin pitch expansion was adjusted based on the assembly expansion to capture the total change in moderator volume.

The results are given in Table II which 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 to help identify trends versus parameter.

As expected, the boron concentration has the largest impact on the TE results. This effect is due to the increase in coolant volume as the pin pitch increases. If the moderator includes a high boron concentration, the total absorptions will increase and the eigenvalue is lower. As the boron concentration decreases, this additional absorption is decreased. Therefore, adding TE to VERA-CS should add a trend in the BOL-EOL boron results for full core problems as the boron concentration decreases through the cycle. The TE effect from the boron is 200 pcm over the range of boron typically found in a reactor cycle. (However, an operating reactor will have feedback which will decrease this effect.)

The pincell geometry type has another fairly large sensitivity to TE, but this is not typically observed in core calculations because all the rods will have similar geometries. The Krško geometry is the most under-moderated geometry in this study, and has the largest sensitivity to TE.

TABLE II. Pincell reactivity differences from thermal expansion (TE - no TE) [pcm].

Category	Set	Ave	Sdev	Min	Max
All		90.9	96.3	-139.2	278.9
Type	BEAVRS	51.5	97.0	-139.2	226.7
	Krško	124.2	89.8	-56.7	278.9
	Surry	90.8	93.1	-91.3	245.7
	WB	97.1	92.5	-85.3	257.0
Enrich.	2.1%	41.5	97.5	-139.2	217.9
	3.1%	98.0	88.5	-74.6	258.8
	4.1%	133.1	79.7	-27.6	278.9
Boron	0	193.4	39.8	-86.0	278.9
	600	87.3	51.3	-39.4	193.6
	1300	-8.1	57.2	-139.2	109.4
Density	den1	73.4	98.7	-139.2	256.1
	den2	89.4	95.8	-120.3	266.3
	den3	109.9	91.7	-95.3	278.9
Tfuel	600	100.7	99.6	-124.9	278.9
	900	90.3	95.8	-131.5	259.7
	1200	81.6	93.4	-139.2	247.4

One unexpected result is the fairly large sensitivity of fuel enrichment to TE. Since accurate fuel rod diameters must be calculated from fuel performance codes, this result suggests that a tighter coupling between the fuel performance code and the neutronics solution might lead to more accurate results.

2. 2D Assemblies (BOL)

The second set of results compares the eigenvalues from a test suite of 1260 single-assembly cases with and without thermal expansion. The test suite includes fourteen different PWR assembly geometries, including 15×15, 16×16, and 17×17 designs by different fuel vendors [13]. Each assembly geometry is run at 81 hot statepoints, including

- three U-235 enrichments (2.1%, 3.1%, and 4.1%),
- three hot coolant densities (inlet, average, and outlet),
- three hot fuel temperatures (600, 900, and 1200 K), and
- three boron concentrations (0, 600, and 1300 ppm).

The test suite includes additional cold statepoints, but these are not relevant for thermal expansion studies.

The assembly cases were run with and without TE to confirm the pincell sensitivities. The differences between eigenvalues with and without TE is shown in Table III.

In addition to the eigenvalue results, the change in pin power was also examined for all cases. These results are shown in Table IV. All of the maximum pin power differences occurred in the outside corner fuel pin. The outside corner fuel pin is affected the most because the assembly gap increases with thermal expansion, and the corner fuel pin will see the largest increase in local moderator volume. A typical increase in assembly gap is from 0.08 cm to 0.141 cm.

TABLE III. Assembly reactivity differences from thermal expansion (TE - no TE) [pcm].

Category	Set	Ave	Sdev	Min	Max
All		52.2	93.4	-129.9	213.9
Enrich.	2.1%	2.4	94.1	-129.9	144.6
	3.1%	58.8	86.1	-66.1	189.1
	4.1%	95.2	77.8	-20.2	213.9
Boron	0	155.7	34.1	88.6	213.9
	600	47.5	44.5	-33.0	119.5
	1300	-46.7	49.0	-129.9	30.6
Density	den1	36.9	96.9	-129.9	193.2
	den2	50.9	94.0	-112.7	202.5
	den3	68.7	90.0	-90.5	213.9
Tfuel	600	61.6	98.1	120.9	213.9
	900	55.2	94.5	-122.0	201.5
	1200	39.7	89.7	-129.9	178.2

TABLE IV. Assembly pin power differences from thermal expansion (TE - no TE) [pcm].

	Ave (%)	Min (%)	Max (%)
Max Difference	2.24	2.69	1.79
RMS Difference	0.70	0.82	0.57

As with the pincell cases, the assembly results show that the largest effect on TE is the boron concentration. There are also smaller sensitivities to geometry type and fuel enrichment.

Sensitivities

A subset of the 2D assembly cases were run to determine the sensitivity of local temperature effects to TE. This study attempts to answer the question of whether or not local temperature changes are important to model.

For this study three assemblies were chosen. The one with most negative reactivity change (low TE case), the nominal case that had a +56.5 pcm change (nominal TE case), and the case with the highest reactivity change (high TE case). The TE of these models used a range of temperatures for the different materials. The summary of the reactivity differences is given in Table V.

The set of rows labeled "Clad" show the result of expanding the fuel cladding at different temperatures. Going from cold conditions to nominal (610 K) show a relatively large change (Row A), and changes ± 30 K around nominal show a smaller eigenvalue change (Rows B and C). These results show that using the exact local clad temperature is not as important as going from cold to hot. This result leads us to the conclusion that we can expand all clad dimensions at the same average clad temperature for the entire core without incurring significant error.

The set of rows labeled "Mod" show the result of expanding the pin pitch and guide tube materials at different temperatures. Here the results are similar to those of "Clad". The largest effect is again going from cold to hot. Local changes on the order of ± 20 K around nominal show smaller changes

TABLE V. Assembly reactivity differences of expansion temperature perturbations (perturb. - ref.) [pcm].

CASE	Expansion Temp	Low	Nominal	High
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	no gap	159.9	-90.9	-174.9

on the order of 10 pcm. Therefore, we conclude using local moderator temperatures for thermal expansion is probably not necessary, and using the core average moderator temperature should be sufficiently accurate.

Lastly there is the fuel category. The most important result here is the bounding "nogap" case where the fuel pellet is expanded out to the cladding. This case suggests that getting the local expansion of the fuel could be important, however, as noted previously, this involves modeling several physics in addition to TE.

3. 3D Whole Core

The third set of test cases is to evaluate the effects of TE on whole-core problems with feedback.

Depletion

To investigate the effects of TE on cycle average boron, the BEAVRS PWR Benchmark Problem [15] was depleted with and without TE included. The depletion was performed at a constant 100% power and all rods out (ARO), and the results are shown in Table VI.

The results from the depletion show that the effects of modeling thermal expansion increase with depletion. From the single-assembly results, we expected the effects of thermal expansion to decrease with decreased boron concentration. However, full-core results have many different competing effects, including thermal-hydraulic feedback, a variety of fuel temperatures, moderator densities, and depletion history effects.

It should be noted that the BEAVRS full-core results are not necessarily consistent with other PWR cores modeled by CASL. This suggests that the full-core results may be plant dependent. Different factors that may affect the specific plant results include rod geometry, inlet temperature, and coolant fraction.

TABLE VI. Critical boron concentration at full-power with and without TE.

Exposure (EFPD)	Boron (ppm) no TE	TE	Diff (ppm)
0	634.8	638.1	3.3
5	588.6	592.6	3.9
15	582.3	585.7	3.4
30	594.5	597.7	3.3
60	576.8	580.2	3.4
90	531.8	535.4	3.7
120	475.6	479.7	4.1
150	412.8	417.6	4.8
180	344.0	349.9	5.9
210	270.6	276.8	6.2
240	192.2	199.0	6.9
270	109.5	117.2	7.7
300	24.1	32.4	8.4

Power Defect

To study the effects of TE on power defect, restart cases were run from the full-power depletions at 0, 150 and 300 EFPD and the critical boron was calculated at 0 power. These results are shown in Table VII

TABLE VII. Critical boron concentration at zero power with and without TE.

Exposure (EFPD)	Boron (ppm) no TE	TE	Diff (ppm)
0	973.0	975.0	-2.5
150	780.3	776.6	-3.7
300	431.5	429.9	-1.6

The results show that the effect of thermal expansion at zero power are opposite to the effect at full-power. This leads to a consistently lower (less negative) power defect with thermal expansion included.

Isothermal Temperature Coefficient

To quantify the effect of TE on Isothermal Temperature Coefficient (ITC), three ITC measurements for the BEAVRS PWR Benchmark problem [15] were modeled with and without TE. The results are shown in Table VIII.

The ITC results demonstrate that modeling TE makes the ITC more positive by 0.2-0.3 pcm/F. These results are consistent with the results of modeling other PWR reactors in CASL.

TABLE VIII. ITC results with and without TE [pcm/F].

ITC Case	No TE	TE
ARO	-2.76	-2.42
Bank C	-2.55	-2.23
Bank C and D	-7.33	-7.02

Baffle Sensitivity

The final numerical result presented is for a full-core PWR model based on the VERA progression problem 7 [14]. This model also includes axial expansion. In this model we also evaluate the TE of the baffle. The effect of TE versus no TE is -5.5 ppm boron, 3.74% max absolute difference in the pin power, 0.69% RMS pin power, a maximum absolute difference in fuel temperature of 14.4 K, and an RMS fuel temperature difference of 4.9 K. This result shows less reactivity difference than the lattice and pincell models, but a higher pin power difference.

In comparing a case with and without TE of the baffle, but TE everywhere else, the Δk difference is 0.15 pcm, the max pin difference and RMS difference are 0.01% in both metrics. This leads us to conclude that expansion of the baffle is not required.

VI. CONCLUSIONS

The methodology for treating thermal expansion in a nuclear reactor is described. The implementation of this methodology in VERA-CS is also summarized. The thermal expansion capability is demonstrated for numerous problems to identify trends in differences in reactivity and the power distribution that result from treating thermal expansion.

In the pincell and lattice cases the maximum reactivity differences observed over a broad range of test problems was 278 pcm in a pincell and 213 pcm for a lattice.

The sensitivities of a lattice to small temperature changes around the nominal temperature were also quantified and these results suggest that capturing the local temperature is not nearly as important as simulating the core average values.

For full-core depletions, the effect of thermal expansion is approximately 10 ppm boron concentration. However, the power defect is noticably less negative and the ITC is more positive by about 0.2-0.3 pcm/F.

In the full core model the maximum local pin power differences was 3.75%, which is larger than the effect predicted from lattice cases, meanwhile the reactivity difference in the full core was less than that observed in the lattice and pincell cases. This is due to the presence of boron in the full core model, where the cases with the maximum reactivity difference for the lattice and pincell had no boron. The full core analysis also showed that the expansion effect on the baffle is not required.

Future work will focus on incorporating more physics into the expansion of the pellet since the fuel pellet diameter includes more effects than thermal expansion with burnup.

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