Computational Heat Transfer Analysis for the Cement Polymerization in a Femoral Implant

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Abstract

A MATLAB simulation has been carried out for the cement polymerization that occurs while implanting an orthopaedic prosthetic in the femur. For this simulation, the heat diffusion equation was taken in axisymmetric coordinates (in two dimensions: z and r). This equation was discretized with second-order centered finite differences for the spatial derivatives to obtain a semi-discrete form of the heat diffusion equation. Next, the simulation performed time marching with the Explicit-Euler method of lines. For a mesh grid resolution of 200 points along the femur and 100 points along the radius of the implant and femur, the maximum bone temperature was determined to be 73 ^{o}C which is hot enough for thermal bone damage to occur. However, this result may not be accurate due to the closeness of the far-field boundaries used in the simulation and the low gird resolutions tested.

Keywords: heat transfer, cement polymerization, hip, femur, implant

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1. Introduction and Problem Definition

An orthopedic prosthetic (or orthopedic implant) is a medical device that is surgically inserted into the human body in order to support a bone or replace a missing joint or bone. One of the techniques to lock the prosthetic in place is cement polymerization which is a chemical reaction that hardens the cement coating of a prosthetic and allows the bone to become anchored to the prosthetic. Furthermore, cement polymerization is an exothermic reaction, one that releases heat to surrounding body tissue. Modelling the heat transfer that occurs in the bone near the implant insertion site is important because damage to bone tissues can occur at elevated temperatures (those between 50 ^{o}C and 70^{o}C) [1]. Therefore, this heat transfer model will provide insight to whether the cement fixation technique is appropriate for inserting an orthopedic prosthetic inside the human body [1].

The scenario that will be modelled is the heat transfer that occurs during the cement polymerization of an orthopedic implant that has been inserted into the femur during hip replacement surgery. Figure 1 illustrates the three components in the model of the implant: the metal stem, the cement (polymethylmethacrylate (PMMA)) and the bone (femur). The model will assume the implant to be axisymmetric along the axis of the stem and therefore, will be described by cylindrical co-ordinates with r being the radial distance from the center of the femur and z being the length along the femur.

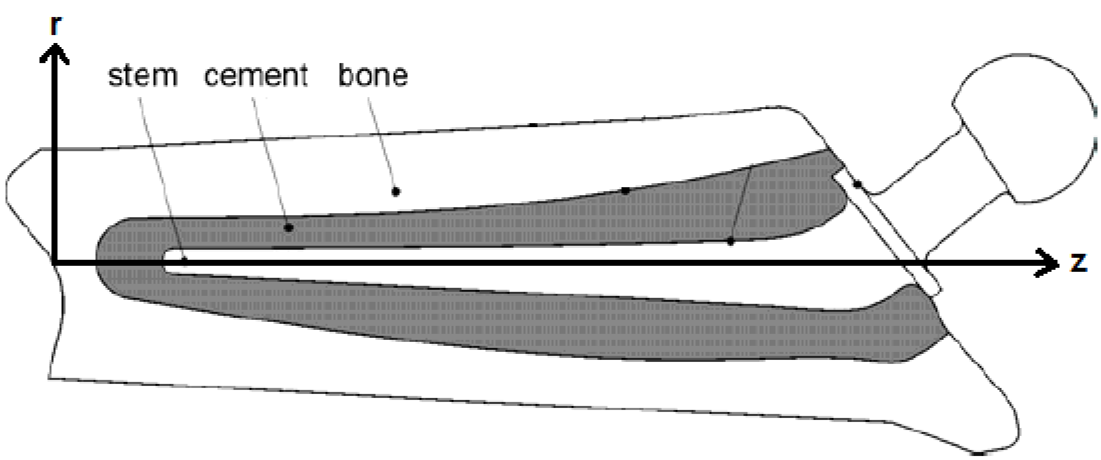

Figure 1. Components of the Femoral Implant Model in Cylindrical Co-ordinates

In this co-ordinate system, Figure 2 defines the domain of heat transfer with the equations of the curves that model the upper cross-sectional slice of the implant in the r-z plane. The domain of the model extends from r = 0 cm to 1.25 cm (the radius of the bone) and from z = 0 cm to 16.25 cm. Taking into consideration the cement, the implant has a total length of 14 cm (from z = 1 cm to 15 cm). Also, there is body tissue from z = 15 cm to z = 16.25 cm and this tissue is assumed to have the same material and thermal properties of bone.

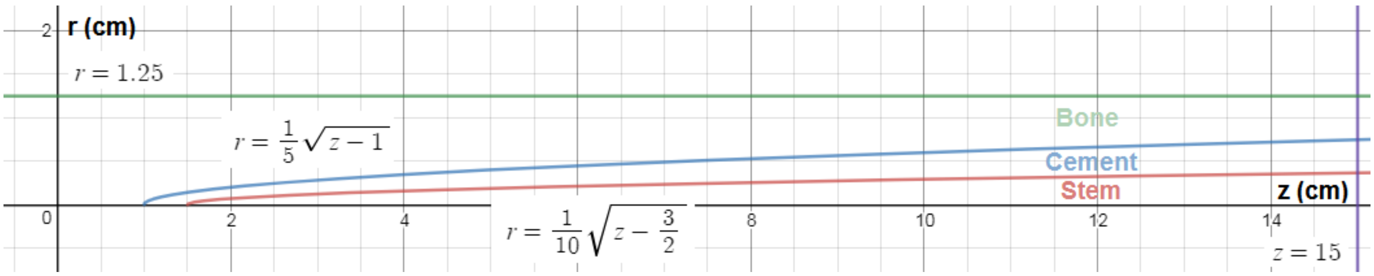

Figure 2. Domain of Heat Transfer with Equations Defined for the Curves of the Stem, Cement and Bone in Cylindrical Co-ordinates

Some additional assumptions include the following:

- There is perfect thermal contact between materials (no thermal contact resistance).
- Surrounding muscle tissue does not contribute to the heat transfer in this model.
- The cement uniformly generates heat per unit volume at a constant rate of 10.615 MW/m^3 for the duration of cement polymerization.
- Cement polymerization takes 15 seconds to complete.
- Time zero is right at the start of cement polymerization.
- Material thermal properties are constant with temperature and direction (numerical values for these properties are listed in Table 1).

Table 1. Thermal Properties of the Materials in the Femoral Implant [1]

	Metal Stem	**Cement**	**Bone**
Thermal Conductivity k [W/(m-K)]	14	0.20	0.45
Specific Heat C [J/(kg-K)]	460	1600	1700
Density ρ [kg/m³]	7800	1100	2000

Ultimately, this model will answer the follow question: what is the temperature distribution in the domain shown in Figure 2 from time zero to sixty seconds after the start of polymerization? By looking at time-evolution of the temperature distribution in the domain, one would be able to determine how the maximum temperature in the bone varies with time to see if thermal bone damage will occur.

2. Continuous Model

For this model, the heat diffusion equation (HDE) is appropriate because it describes the variation of temperature in space and time. Since three materials of different thermal properties are in the model, the HDE needs to be split into three equations for the stem (s), cement (c), and bone (b) and body tissue (t) as respectively shown in Equations 1, 2 and 3,

$$\rho_s C_s \frac{\partial T}{\partial t} = \vec{\nabla} \cdot \left(k_s \vec{\nabla} T\right) \qquad if\ r, z \in D_s \tag{1}$$

$$\rho_c C_c \frac{\partial T}{\partial t} = \vec{\nabla} \cdot \left(k_c \vec{\nabla} T\right) \qquad if\ r, z \in D_c \tag{2}$$

$$\rho_b C_b \frac{\partial T}{\partial t} = \vec{\nabla} \cdot \left(k_b \vec{\nabla} T\right) + \dot{q} \qquad if\ r, z \in D_b \cup D_t \tag{3}$$

where ρ, C and k are the material and thermal properties for the three materials as defined in Table 1 and T is the temperature which is a function of z, r and time (t).

These equations describe the thermal energy balance law during heat transfer due to conduction. The $\rho C \frac{\partial T}{\partial t}$ term represents the change of thermal energy in each material with respect to time which must balance the heat fluxes ($k\vec{\nabla} T$) crossing the boundaries of each material and $\dot{q}$ the rate of thermal energy generated within a material per unit volume. Furthermore, these equations are parabolic, and they describe thermal energy spreading in all directions at infinite speed.

D_s, D_c, D_b and D_t are the domains of the stems, cement, bone and body tissue which are given by Equations 4, 5, 6 and 7 respectively.

$$D_s = \left\{z, r \in \mathbb{R} \,|\, 1.5\ cm\ \le z\ < 15\ cm\ \cap\ 0 \le \mathrm{r} \le 0.1\sqrt{z - 1.5}\ \right\} \tag{4}$$

$$D_c = \begin{Bmatrix} z, r \in \mathbb{R} \,|\, (1\ cm\ \le z < 1.5\ cm\ \cap\ 0 \le \mathrm{r}\ \le 0.2\sqrt{z-1})\ \cup \\ (1.5\ cm \le z < 15\ cm\ \cap\ 0.1\sqrt{z-1.5} < r\ \le\ 0.2\sqrt{z-1}) \end{Bmatrix} \tag{5}$$

$$D_b = \begin{Bmatrix} z, r \in \mathbb{R} \,|\, (0\ cm\ \le z < 1\ cm\ \cap\ 0 \le \mathrm{r}\ \le 1.25\ cm)\ \cup \\ (\ 1\ cm \le z < 15\ cm\ \cap\ 0.2\sqrt{z-1} < r\ \le 1.25\ cm) \end{Bmatrix} \tag{6}$$

$$D_t = \{z, r \in \mathbb{R} \,|\, 15\ cm\ \le z\ \le 16.25\ cm\ \cap\ 0 \le \mathrm{r} \le 1.25\ cm\} \tag{7}$$

Equation 3 is the most general of the three HDEs. Expanding Equation 3 by taking the divergence of the thermal conductivity multiplied by the gradient of temperature produces Equation 8,

$$\rho C \frac{\partial T}{\partial t} = \frac{k}{r} \frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r}\right) + \frac{k}{r^2} \frac{\partial}{\partial \theta}\left(\frac{\partial T}{\partial \theta}\right) + k \frac{\partial}{\partial z}\left(\frac{\partial T}{\partial z}\right) + \dot{q} \tag{8}$$

where material and thermal properties are for an arbitrary material, and $\frac{\partial T}{\partial r}$, $\frac{\partial T}{\partial \theta}$ and $\frac{\partial T}{\partial z}$ are the temperature changes in the r, θ and z directions.

Because this model is axisymmetric, $\frac{\partial T}{\partial \theta} = 0$. Making the axisymmetric simplification, applying the chain rule on the first term on the right-hand side, and dividing both sides by ρC yields Equation 9,

$$\frac{\partial T}{\partial t} = \frac{\alpha}{r}\frac{\partial T}{\partial r} + \alpha\left(\frac{\partial^2 T}{\partial z^2} + \frac{\partial^2 T}{\partial r^2}\right) + S \tag{9}$$

where α, thermal diffusivity [m^2/s], is defined by Equation 10 and S, the heat source [K/s] (which is in the cement only) is defined by Equation 11.

$$\alpha = \frac{k}{\rho C} \tag{10}$$

$$S = \frac{\dot{q}}{\rho C} \tag{11}$$

From literature, a heat generation of 10.615 MW/m^3 in the cement was found to be appropriate for this kind of heat transfer problem [1]. Applying Equation 11 for the cement gives a heat source of about 6.03 K/s in the cement; the heat source is zero in the stem, bone and body tissue.

In this model, the outer boundaries in contact with bone or body tissue are set to be at body temperature and the lower boundary (the boundary along the z axis) in contact with parts of the implant are set to be at ambient temperature as described by Equations 12 and 13:

$$T(0, r, t) = T(r, 16.25\ cm, t) = T(z, 1.25\ cm, t) = 37°C\ or\ 310\ K \tag{12}$$

$$T(z, 0, t) = \begin{cases} 310\ K & if\ 0 \le z < 1\ cm\ \cup\ 15\ cm \le z \le 16.25\ cm \\ 295\ K & if\ 1\ cm\ \le z < 15\ cm \end{cases} \tag{13}$$

Equation 14 provides the initial conditions for this problem; the stem and cement start at ambient temperature and the bone and body tissue start at body temperature.

$$T(z, r, 0) = \begin{cases} 295\ K & if\ r, z \in D_s \\ 295\ K & if\ r, z\ \in D_c \\ 310\ K & if\ r, z \in D_b \cup D_t \end{cases} \tag{14}$$

In this model, the following effects have been neglected:

- Thermal contact resistance at the interfaces between materials
- Variation in thermal properties with temperature
- Temporal variation in the heat generated in the cement per unit volume
- Temporal variation in the temperature of the boundary along the z-axis

The effects of thermal contact resistance and changing thermal properties with time may have noticeable effects on the rate of conductive heat transfer. Neglecting thermal contact resistance means that this model assumes that heat moves more readily through the system than it would in reality. Also, thermal conductivity may increase or decrease with temperature meaning that the model may respectively underestimate or overestimate the rate of heat transfer while the heat source is increasing the temperature of the system in time.

Furthermore, the heat generated in the cement depends on the fraction of cement polymerization complete and the rate of cement polymerization which both depend on temperature (and thus, time) [1]. This model assumes a constant heat generation for a specified period of time which may produce a different total amount of heat produced than in the case where the effects of the polymerization reaction on the heat generation rate are considered. Therefore, the results of this model may not be perfectly realistic.

The segment of the implant along the z-axis is assumed to always be at ambient temperature. However, while the cement is producing heat, the temperature of the middle of the implant along the z-axis changes. Since this segment along the z-axis is small compared to the entire domain, assuming a constant ambient temperature in that segment will have negligible effects on the results.

3. Discrete Model

A semi-discrete approach has been used to discretize the continuous model:

1. Discretize the spatial derivatives.
2. Express the temporal derivative in its continuous form in terms of the discretized spatial derivatives (in other words, obtain the semi-discrete form of the rate of temperature change).
3. Choose a method to time march using the method of lines.
4. Choose a time-step size for time marching that ensures the stability of the solution for the temperature distribution.
5. Time march.

The spatial derivatives in Equation 9 are discretized with centered second-order finite differences which are described by Equations 15, 16 and 17.

$$\frac{\partial T}{\partial r} = \frac{T_{i,j+1} - T_{i,j-1}}{2\Delta r} \tag{15}$$

$$\frac{\partial^2 T}{\partial r^2} = \frac{T_{i,j-1} - 2T_{i,j} + T_{i,j+1}}{\Delta r^2} \tag{16}$$

$$\frac{\partial^2 T}{\partial z^2} = \frac{T_{i-1,j} - 2T_{i,j} + T_{i+1,j}}{\Delta z^2} \tag{17}$$

A two-dimensional rectangular mesh with a chosen numbers of points in "i" and "j" has been created in the MATLAB code for this model which can be found in Appendix A. Indices "i" and "j" represent the z and r co-ordinates respectively of a point (i, j) in the r-z plane. $T_{i,j}$ is the temperature at point (i, j). The temperatures at the immediate top and bottom neighbouring points to point (i, j) are denoted as $T_{i,j+1}$ and $T_{i,j-1}$, whereas the temperatures of the immediate left and right neighbouring points are denoted as $T_{i-1,j}$ and $T_{i+1,j}$.

It is important to note that all of the points in the mesh are inside the outer boundaries of the domain which means that none of these points lie along these boundaries. For computations that occur at points along the top, bottom, left or right outer edges of the rectangular mesh, the temperatures along the boundaries of the system must be taken as the top, bottom, left or right neighbouring temperatures respectively.

Substituting Equations 15, 16 and 17 (the discrete spatial derivatives) in Equation 9 yields Equation 18, the semi-discrete form of the rate of temperature change,

$$\left(\frac{\partial T}{\partial t}\right)_{i,j}^{(n)} = \frac{\alpha}{2r_{i,j}\Delta r}\left(T_{i,j+1}^{(n)} - T_{i,j-1}^{(n)}\right) + \frac{\alpha}{\Delta z^2}\left(T_{i-1,j}^{(n)} - 2T_{i,j}^{(n)} + T_{i+1,j}^{(n)}\right) + \frac{\alpha}{\Delta r^2}\left(T_{i,j-1}^{(n)} - 2T_{i,j}^{(n)} + T_{i,j+1}^{(n)}\right) + S \tag{18}$$

where $r_{i,j}$ is the r co-ordinate of point (i, j). The spacing between points on the mesh are given by Δz and Δr which are described by Equations 19 and 20,

$$\Delta z = \frac{z_{max} - z_{min}}{n_z + 1} \tag{19}$$

$$\Delta r = \frac{r_{max} - r_{min}}{n_r + 1} \tag{20}$$

where z_{max} and z_{min} are the upper and lower limits of z, and r_{max} and r_{min} are the upper and lower limits of r. Recall that z ranges from 0 to 16.25 cm and r ranges from 0 to 1.25 cm. Since the mesh does not have points along the outer boundaries of the domain, in each of the z and r directions, there is one more interval than the number of points in z and r (denoted by n_z and n_r respectively).

In Equation 18, there is a superscript of "(n)" for every term. This superscript indicates the timestep (or in other words, the point in time) at which each term at point (i, j) is evaluated.

Equation 21 shows how the time [s] at the n-th timestep is calculated,

$$t^{(n)} = t^{(n-1)} + \Delta t \tag{21}$$

where $t^{(n-1)}$ is the time of the previous timestep and Δt is the difference in time from one timestep to the next; $t^{(0)}$ is the initial time which is set to zero.

For time-marching, the Explicit Euler method of lines is used as shown in Equation 22.

$$T_{i,j}^{(n+1)} = T_{i,j}^{(n)} + \Delta t \left(\frac{\partial T}{\partial t}\right)_{i,j}^{(n)} \tag{22}$$

With this method, at every timestep (n), the temperature at points (i, j) one timestep in the future (n+1) is determined by creating a line segment of slope $\left(\frac{\partial T}{\partial t}\right)_{i,j}^{(n)}$ that runs from the temperature at the current timestep (n) to the temperature one timestep in the future. The slope is the temperature rate of change at the current time step. Using this method iteratively from the initial to the final simulation times produces a solution of many line segments for the temperature distribution. This segmented solution can be visualized on a graph of temperature vs. time.

It can be shown through a von-Neumann stability analysis that if one were to take the linear diffusion equation and use second-order centered finite differences for the spatial derivatives and time march with the Explicit-Euler method, one would find the solution to be conditionally stable. Here, it is possible for one to find a Δt that produces a stable solution. A stable solution is one whose amplitude stays constant or decreases from one timestep to the next. In some cases, certain combinations of finite-difference schemes and time-marching methods yield unstable solutions which are undesirable. An unstable solution is one whose amplitude increases from one timestep to the next which causes the solution to go to infinity.

Therefore, in order to obtain a stable solution for the heat diffusion equation in this model, second-order centered differences in space and the Explicit-Euler time marching method were used.

From the von-Neumann stability analysis for the linear diffusion described earlier, it was found that the solution is stable if Δt is in the range given by Equation 23,

$$0 < \Delta t \leq \frac{\Delta^2}{2\alpha} \tag{23}$$

where Δ is the spacing between points on the line of the direction of interest in case of the linear diffusion equation.

In order for Δt to fall in this range, a safety factor in between 0 and 1, called the CFL number, is chosen. Equation 24 shows how Δt is calculated for this model.

$$\Delta t = CFL \frac{\Delta_{min}^2}{2\alpha_{max}} \tag{24}$$

In this model, CFL is set to 0.8. Considering the worst-case scenario for choosing a Δt that would yield a stable solution, Δ_{min} is the minimum of Δ_z and Δ_r, and α_{max} is the maximum of the stem, cement and bone thermal diffusivities.

In the MATLAB simulation, these most important computations of the discrete model are done in the following order:

1. Find the rate of temperature change at the initial time for all the points on the mesh using Equation 18.
2. Time march to find the temperatures one timestep in the future at all points using Equation 22.
3. Increment the timestep with Equation 21.
4. Repeat steps 1 to 3 until the final time is reached.

4. Resolution Study

For this heat transfer problem, to determine the appropriate mesh size and timestep size, a low-resolution grid was first simulated and then, the resolution was refined twice by doubling the number of points in z and r each time. Table 2 presents the characteristics of the three simulations in this grid-refinement study.

Table 2. Characteristics of the Grid-Refinement Study of the Heat Transfer Model

Simulation	Resolution (n_z x n_r)	Δt [s]	Number of Iterations	Computation Time [s]
1	50 x 25	0.0237	2533	6 min, 18 sec
2	100 x 50	0.00616	9743	26 min, 1 sec
3	200 x 100	0.00157	38212	2h, 17 min, 38 sec

For simulation 1 (the coarsest mesh), the contour maps showing the temperature distributions of the implant at time zero, at the time of the absolute maximum temperature in the implant and at the final time (60 seconds) are shown in Figures 3, 4 and 5 respectively.

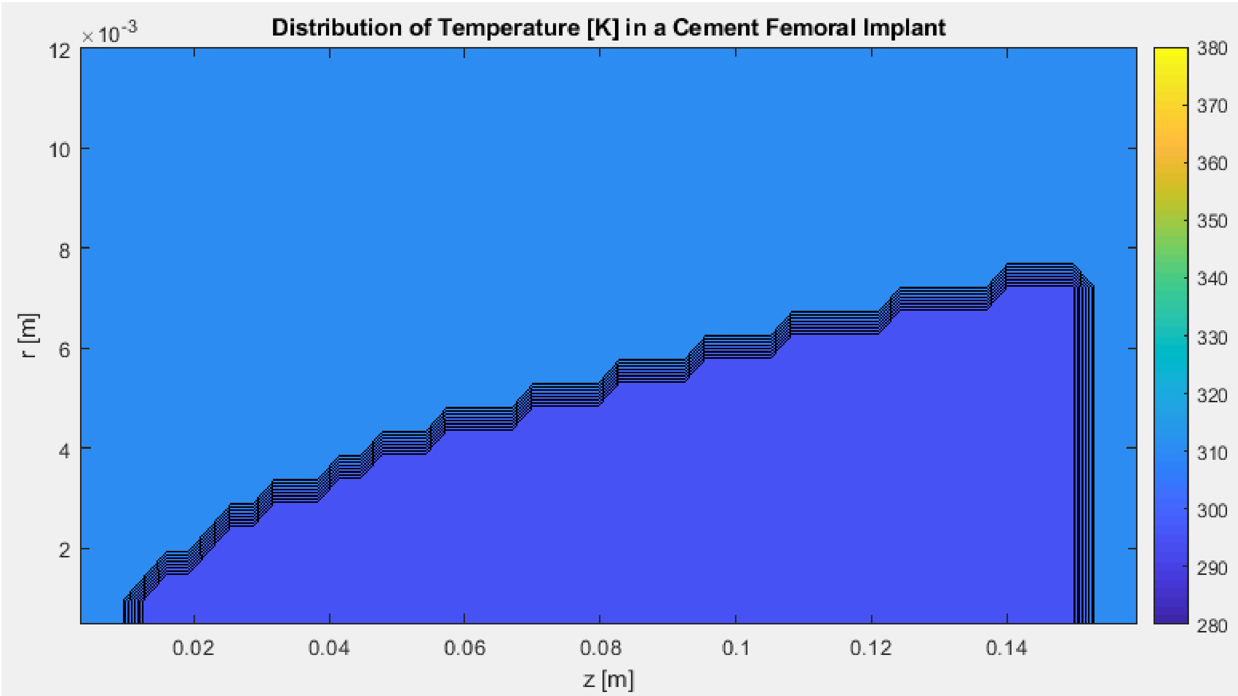

Figure 3. Initial Temperature Distribution [K] in the Femoral Implant for (n_z x n_r) = (50 x 25)

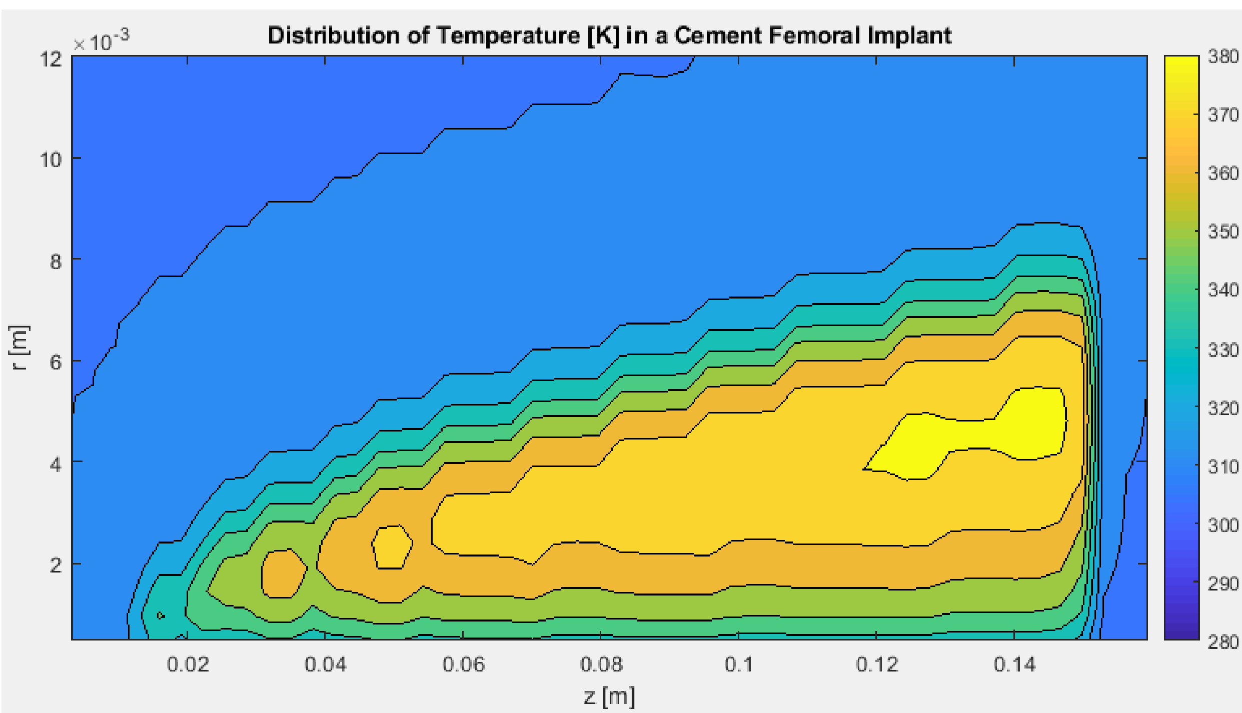

Figure 4. Temperature Distribution [K] in the Femoral Implant for (n_z x n_r) = (50 x 25) at the Time of the Absolute Maximum Temperature in the Entire Implant

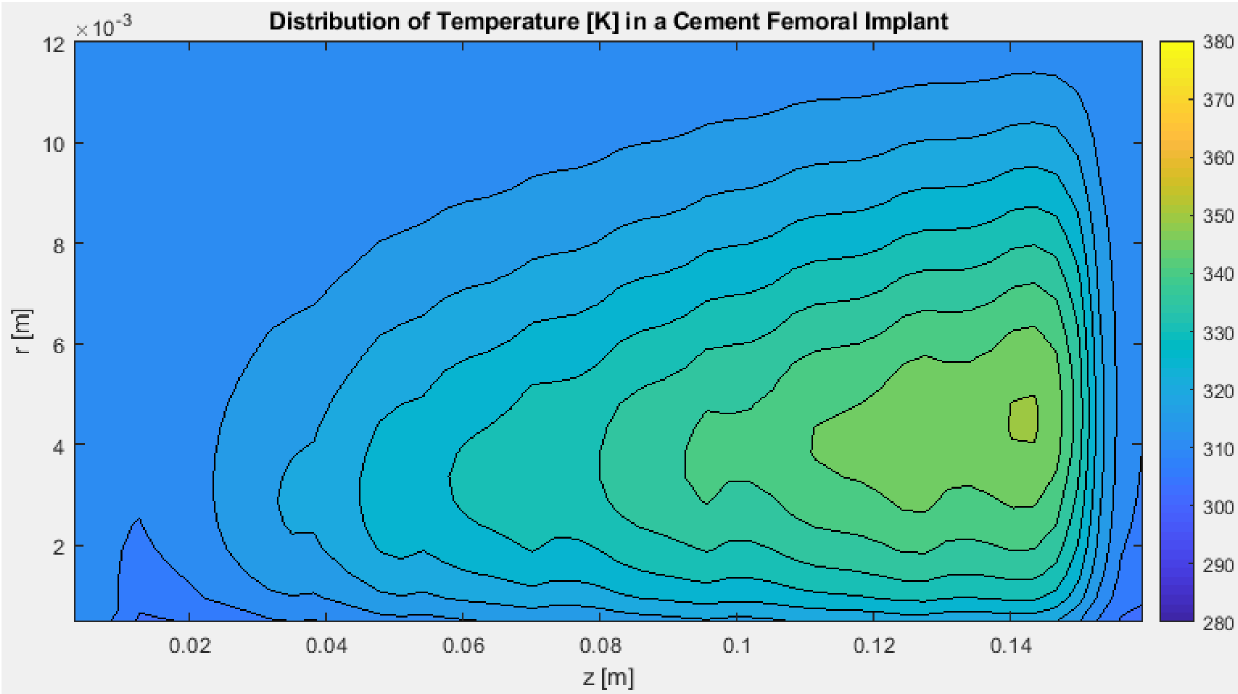

Figure 5. Final Temperature Distribution [K] in the Femoral Implant for (n_z x n_r) = (50 x 25)

In Figures 3, 4 and 5, the curves defining the regions of different temperatures are jagged and unsmooth. At time zero, one would expect the curve defining the initial temperature of the implant to be smooth like the curve of the root function defined for the cement in Figure 2. This jaggedness is an indication the grid size and timestep size in simulation 1 may not be appropriate to obtain an accurate answer for the temperature distribution from 0 to 60 sec. However, to confirm that this grid size is too coarse for an accurate answer, temperature values would need to be compared from one resolution to the next. These comparisons are done later in this section.

In simulation 2, the resolution has been doubled from simulation 1 and the contour maps of the temperature distributions at the same times of interest are illustrated in Figures 6, 7 and 8.

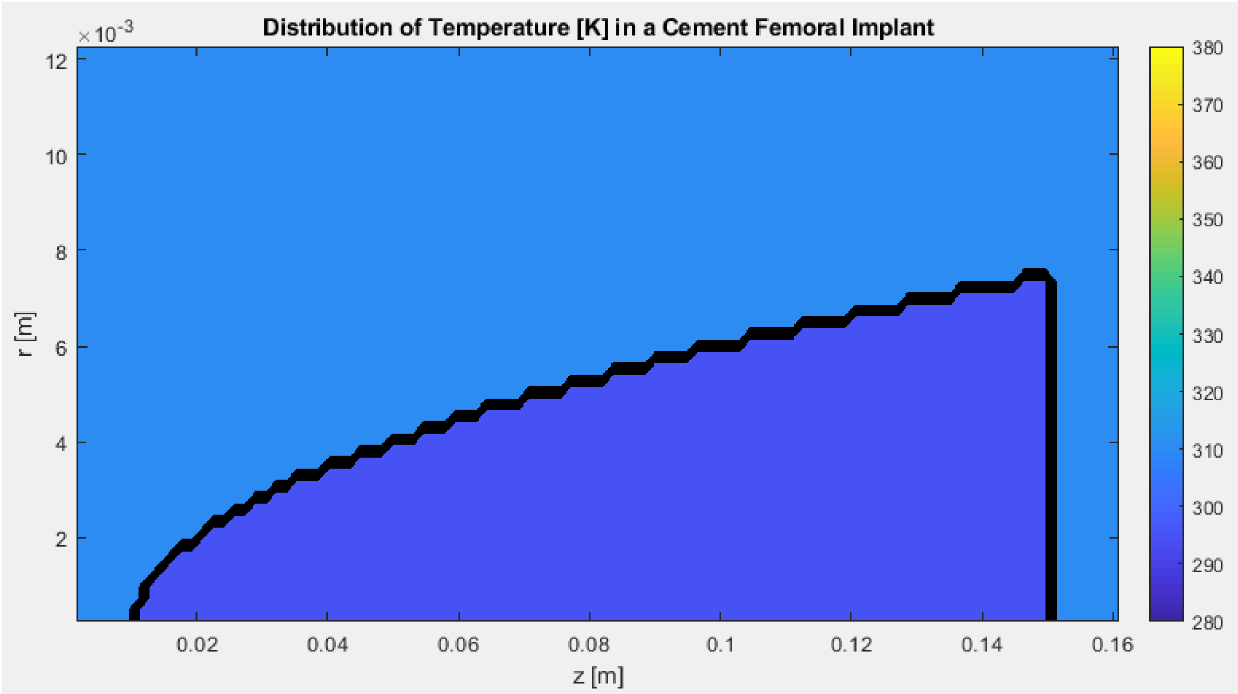

Figure 6. Initial Temperature Distribution [K] in the Femoral Implant for (n_z x n_r) = (100 x 50)

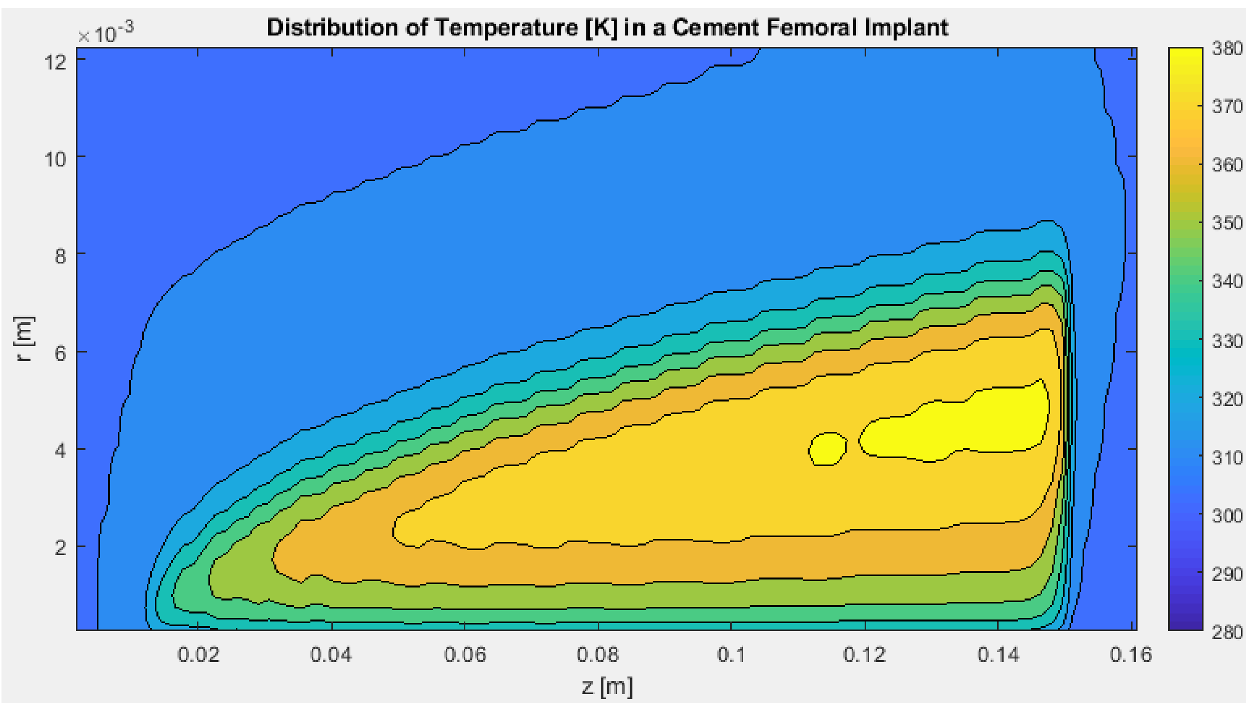

Figure 7. Temperature Distribution [K] in the Femoral Implant for (n_z x n_r) = (100 x 50) at the Time of the Absolute Maximum Temperature in the Entire Implant

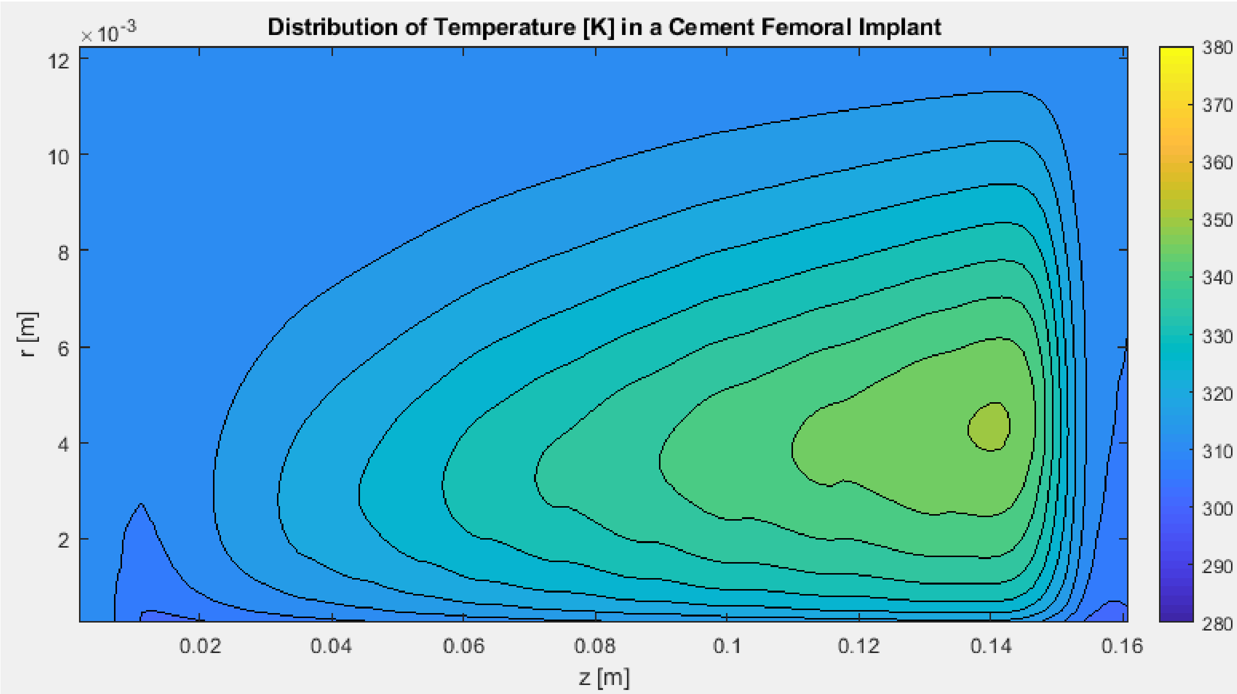

Figure 8. Final Temperature Distribution [K] in the Femoral Implant for (n_z x n_r) = (100 x 50)

Figures 6, 7 and 8 show smoother curves defining regions of different temperatures. Visually, the temperature distributions are similar from simulation 1 to simulation 2; however, this is not conclusive evidence that any of the resolutions and timesteps in those two simulations provides an accurate answer. Simulation 3 provides more information.

Doubling the resolution again produces Figures 9, 10 and 11 which are again, the contour maps of the temperature distributions of the times of interest.

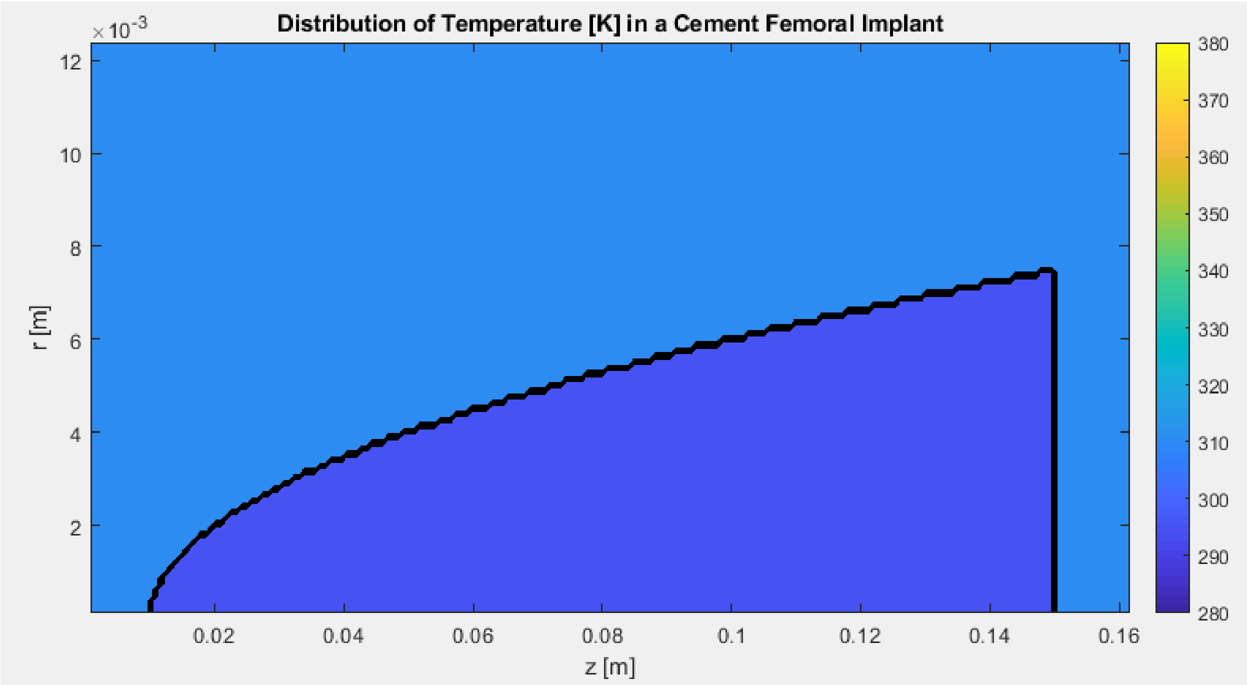

Figure 9. Initial Temperature Distribution [K] in the Femoral Implant for $(n_z \text{ x } n_r)$ = (200 x 100)

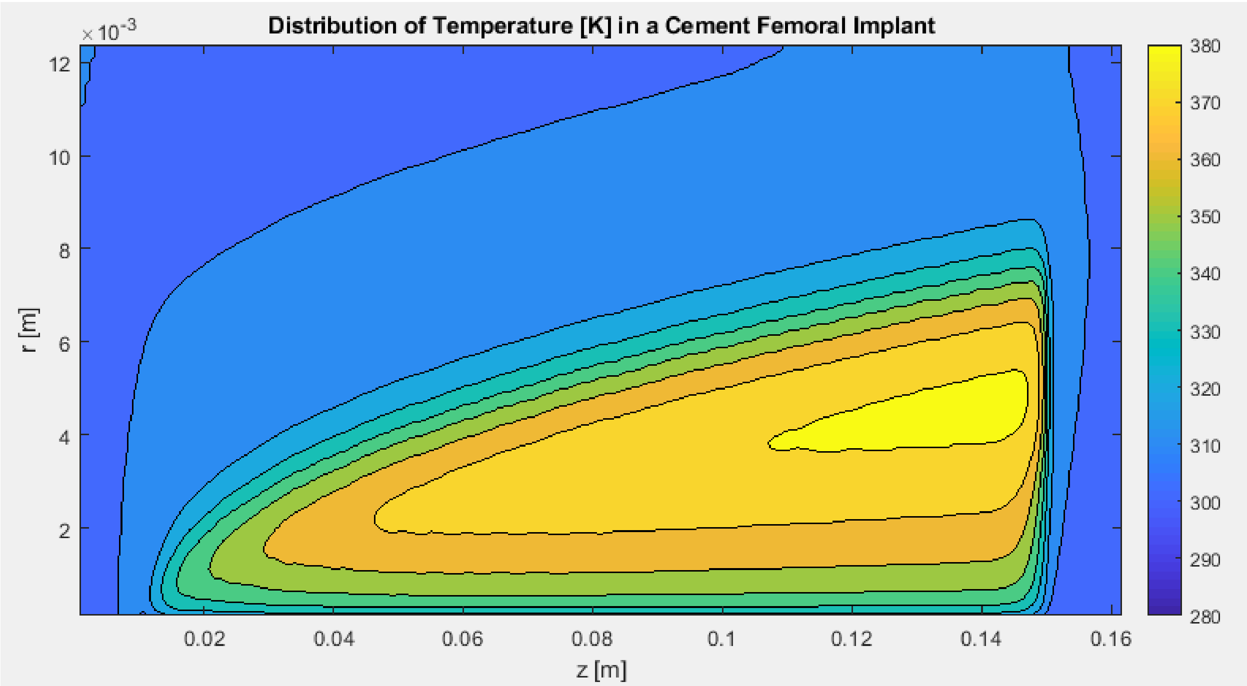

Figure 10. Temperature Distribution [K] in the Femoral Implant for $(n_z \text{ x } n_r)$ = (200 x 100) at the Time of the Absolute Maximum Temperature in the Entire Implant

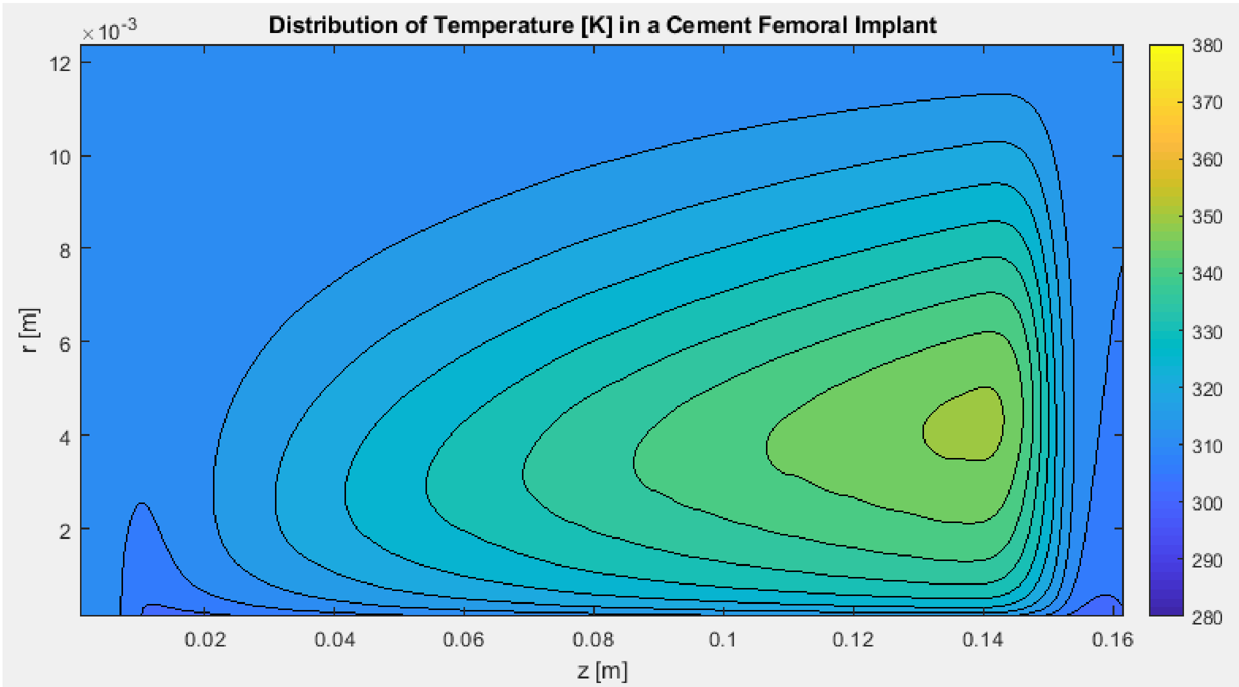

Figure 11. Final Temperature Distribution [K] in the Femoral Implant for (n_z x n_r) = (200 x 100)

Compared to simulations 1 and 2, simulation 3 defines different temperatures of different regions with curves that are much smoother than in simulations 1 and 2. In addition, the temperature distributions in simulations 2 and 3 are similar which is an indication that a resolution of (200 x 100) and 0.00157 s could be acceptable.

Figure 11 shows the final temperature to be approximately 320 K along most of the edges of the far-field boundary when it is expected to stay constant at 310 K (body temperature). Therefore, the far-field boundaries are close enough to affect the results and they would need to be set further away from the cement heat source in order for more reliable results to be obtained. In a future simulation, one can set the far-field boundaries to be 5 cm away from all edges of the hip implant.

In this heat transfer problem, the goal is to use the temporal temperature distribution to determine how the maximum bone temperature varies with time. For all three resolutions tested, the timed-based variation in bone temperature is shown in Figure 12.

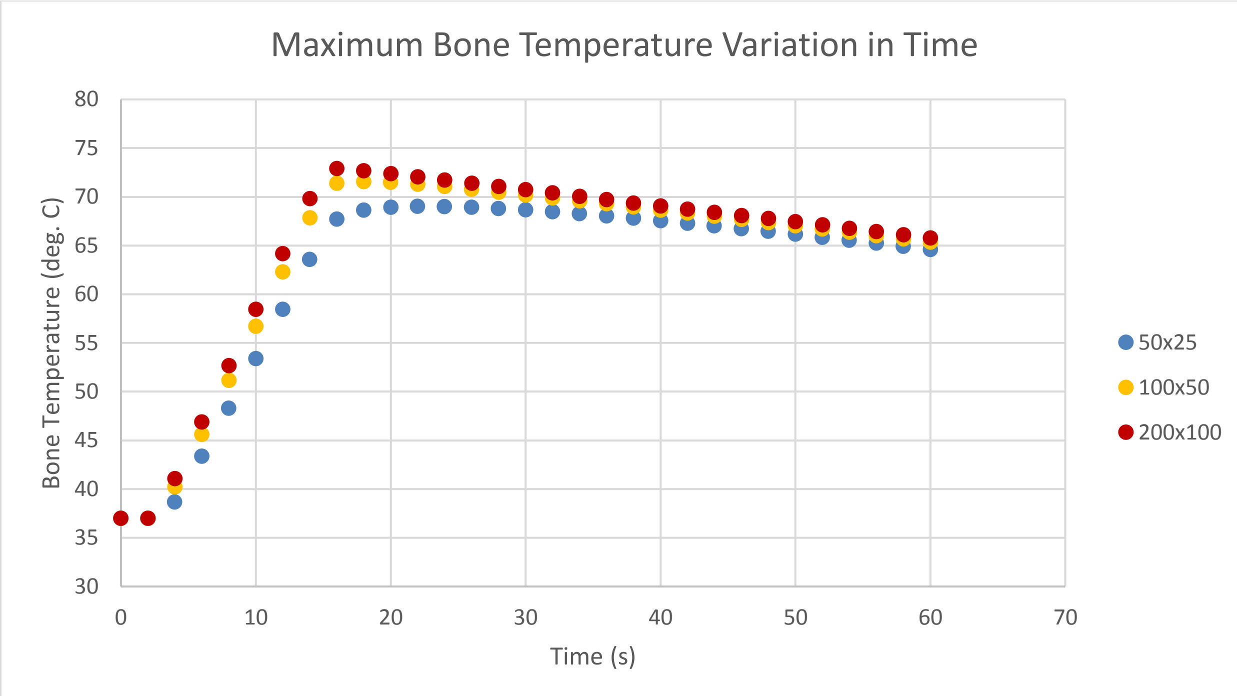

Figure 12. Maximum Bone Temperature (^{o}C) at Different Points in Time for Resolutions of (50 x 25), (100 x 50) and (200 x 100)

From one resolution to the next, there are noticeable differences in bone temperature at a specific point in time. Thus, I would not consider a resolution of 200 x 100 to trust the answer provided by simulation 3. Nevertheless, the difference in maximum bone temperatures is smaller between resolutions of (100 x 50) and (200 x 100) than between resolutions of (50 x 25) and (100 x 50), so a resolution of (400 x 200) would likely produce a trustable answer. However, given the computational resources available, a simulation of (400 x 200) would have taken more than twelve hours to complete. By the time the (200 x 100) simulation was done, I did not have enough time to proceed with the (400 x 200) simulation.

5. Results and Discussion

It is most practical to solely interpret the results of the simulation with the finest resolution (simulation 3).

Figure 9 shows the initial temperature distribution with the implant being at ambient temperature (295 K) and the surrounding bone and body tissue being at body temperature (310 K). This distribution is what one would expect right before the start of cement polymerization.

Moreover, Figure 10 shows that the absolute maximum temperature of the entire implant during the simulation was approximately 380 K (107 ^{o}C). This temperature occurs right at the end of cement polymerization which is at 15 seconds. The purpose of obtaining the contour plot at time of the absolute maximum temperature was to determine if the chosen constant cement heat source term and duration of cement polymerization were realistic. Stanczyk and Telega (2002) found that during this chemical reaction, the bone surface temperature can rise up to over 100 ^{o}C within the cement domain [1]. Therefore, the selected cement heat generation term of 10.615 MW/m^3 over a duration of 15 seconds seems to have been a reasonable selection for the source term.

Figure 10 also demonstrates that the source of heat is most effective towards the right of the domain. This occurs because the curves defining the stem and the cement are close together towards the left of the domain and become more separated as one moves to the right of the domain as illustrated in Figure 2. Thus, the area of cement is greatest near right boundary of the domain, producing the absolute maximum temperature of 380 K at the location shown in Figure 10. The heat diffusion equation describes heat spreading in all directions which is clearly indicated by the gradually decreasing temperature gradient around the cement. From the cement moving outward along r, the temperature gradually decreases from 380 K to 370 K to 360 K and eventually to 310 K. In addition, the heat diffusion equation represents heat spreading at infinite speeds, so the effects of the cement heat source were instantaneously experienced at all points in the domain.

Figure 11 demonstrates that after the cement curing was completed, heat began to dissipate from the cement to the stem, bone and body tissue. At the end of the simulation, the absolute maximum temperature was around 350 K and most of the bone was at a temperature of 320 K. Figures 10 and 11 show the effect of the far-field boundaries being too close. At 15 seconds, the temperature is 310 K (body temperature) at most parts of the far-field boundaries. However, at 60 seconds the far-field boundary temperature has increased to 320 K meaning that the domain of simulation was not large enough for all the heat to properly be dissipated into the body. This presents a source of error because in this case, the thermal energy is being trapped inside of a small domain causing the temperatures within the domain to higher than they would be in reality.

In Figure 12, the maximum bone temperature results have been presented in ^{o}C so that they are easily comparable to literature data. For all three resolutions tested, the bone temperature starts at body temperature (37 ^{o}C) and increases during cement curing when the cement is releasing heat. The maximum bone temperature occurs at approximately 16 seconds which is one second after the end of curing and one second after the occurrence of the absolute maximum temperature. The maximum bone temperatures are 68 ^{o}C, 71 ^{o}C and 73 ^{o}C for resolutions of (50 x 25), (100 x 50) and (200 x 100) respectively. These numbers reinforce the fact that these resolutions are not refined enough for an accurate answer because these temperatures are separated by more than 1 ^{o}C. In bone, collagen protein denaturation takes place in the temperature range of 56 to 70 ^{o}C and a temperature of 70 ^{o}C is believed to kill bone cells instantly [1]. Therefore, these results show that thermal bone damage will happen if the femoral implant is installed under the conditions assumed in this model. However, the closeness of the far-field boundaries and low simulation resolution are sources of error that have caused the temperatures to be higher than expected.

6. Conclusions

After simulating the heat transfer during cement polymerization in a hip implant, the following observations were made:

1. The maximum absolute temperature of the implant in cement polymerization is 107 ^{o} C.
2. The maximum bone temperature during this process is 73 ^{o}C.
3. These results are likely inaccurate due to the closeness of the far-field boundaries and the low resolutions of the simulations.

Reference

[1] Stanczyk, M., & Telega, J. (2002). Modelling of heat transfer in biomechanics – a review Part II. Orthopaedics. *Acta of Bioengineering and Biomechanics, 4*(2), 3-33.

Appendix A – MATLAB Code for the Heat Transfer Simulation

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%                                                                          %
%                       MCG 4139 - Final Project                           %
%                 Code written by Michael Botros 8327615                   %
%                 Code written for Dr. James McDonald                      %
%                           April 26th, 2019                               %
%                                                                          %
%               Heat Transfer in a Cement Femoral Implant                  %
%                                                                          %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Notes about the code:
% 1. "i" will represent the z direction and
%    "j" will represent the r direction.
% 2. All dimensions and properties are expressed in SI units.

function MCG4139FinalProjectMBotros

    % Initialize cement polymerization time and total simulation time
    polymerization_time = 15.0;
    final_time = 60.0;

    % Number of points in the z and r directions
    nz = 200;
    nr = 100;

    % Safety factor for the time step to be small enough for stability
    CFL = 0.8;

    % Boundaries of the simulation (units of cm have been converted to m)
    zmin = 0.0;
    zmax = 0.1625;
    rmin = 0.0;
    rmax = 0.0125;

    % Boundary temperatures (in Kelvin)
    T_bound_stem   = 295.0;
    T_bound_cement = 295.0;
    T_bound_bone   = 310.0;
    T_bound_tissue = 310.0;

    % Material thermal properties
    ks = 14.0;
    kc = 0.20;
    kb = 0.45;
    Cs = 460.0;
    Cc = 1600.0;
    Cb = 1700.0;
    rho_s = 7800.0;
    rho_c = 1100.0;
    rho_b = 2000.0;

    % Heat generated per unit volume in the cement
```

```
    q_gen = 10.615e6; % (units of MW/m^3 have been converted to W/m^3)

    % Heat source
    Source = q_gen/(rho_c*Cc); % (in Kelvin/second)

    %% Initialize

    delta_z = (zmax-zmin)/(nz+1);
    delta_r = (rmax-rmin)/(nr+1);
    delta = min(delta_z,delta_r);

    [r,z] = meshgrid(rmin+delta_r:delta_r:rmax-
delta_r,zmin+delta_z:delta_z:zmax-delta_z);
    T = initial_conditions(nz,nr,z,r);

    alpha_s = ks/(rho_s*Cs);
    alpha_c = kc/(rho_c*Cc);
    alpha_b = kb/(rho_b*Cb);
    alpha = maximum(alpha_s,alpha_c,alpha_b);

    delta_t = CFL*((delta^2)/(2*alpha));

    time = 0.0;
    iteration = 0;

    % Used to store maximum bone temperatures (T) at certain points in time
(t)
    numpoints_t = 31;
    numpoints_T = numpoints_t;
    sampling_dt = final_time/(numpoints_t-1);
    counter = 1; % Used to keep track of how many data points have been
stored
    t_storage = zeros(numpoints_t,1);
    T_storage = zeros(numpoints_T,1);

    %% Time march
    while time < final_time

        % Initialize rate of temperature change
        dTdt = zeros(size(T));

        for i = 1:nz
          for j = 1:nr

            % Find T at the "middle" node
            Tm = T(i,j);

            % Find T at the "left" neighbour
            if i > 1
              Tl = T(i-1,j);
            else
              Tl = T_bound_bone;
            end
```

```
            % Find T at the "right" neighbour
            if i < nz
              Tr = T(i+1,j);
            else
              Tr = T_bound_tissue;
            end

            % Find T at the "bottom" neighbour
            if j > 1
                Tb = T(i,j-1);
            elseif z(i,j) >= 0.0 && z(i,j) < 0.01
                Tb = T_bound_bone;
            elseif z(i,j) >= 0.01 && z(i,j) < 0.015
                Tb = T_bound_cement;
            else
                Tb = T_bound_stem;
            end

            % Find T at the "top" neighbour
            if j < nr
              Tt = T(i,j+1);
            else
              Tt = T_bound_bone;
            end

            % Find z and r co-ordinates
            z_ij = z(i,j);
            r_ij = r(i,j);

            % Get thermal diffusivity based on location in domain
            a = get_thermal_diffusivity(z_ij,r_ij,alpha_s,alpha_c,alpha_b);

            % Get heat source based on whether or not cement polymerization
            % is still occurring and based on location in domain
            if time < polymerization_time
              S = get_heat_source(z_ij,r_ij,Source);
            else
              S = 0;
            end

            % Heat diffusion equation with centered finite differences for
            % the spatial derivatives
            dTdt(i,j) = (a/(2*(r(i,j))*delta_r))*(Tt-Tb) ...
                        + (a/(delta_z^2))*(Tl-(2*Tm)+Tr) ...
                        + (a/(delta_r^2))*(Tb-(2*Tm)+Tt) + S;

          end
        end

        % Find maximum bone temperatures and store them in memory
        T_max = get_max_bone_temperature(nz,nr,z,r,T);
        if time > (sampling_dt*(counter-1) - delta_t) && time <
(sampling_dt*(counter-1) + delta_t)
            t_storage(counter) = time;
            T_storage(counter) = T_max;
```

```
            counter = counter + 1;
        end

        % Plot temperature field
        if time == 0
            fig_num = 1;
            produce_plot(fig_num,z,r,T);
        end
        fig_num = 2;
        produce_plot(fig_num,z,r,T);

        % Update (Explicit-Euler time-marching)
        T = T + delta_t*dTdt;
        iteration = iteration +1;
        time = time + delta_t;
        if time > final_time
            delta_t = time - final_time;
            time = final_time;
        end

        %% Output update every time step
        disp(sprintf('timestep %i, time = %0.5e, delta_t = %0.5e, Max bone T
= %0.7f degrees Celsius', ...
                     iteration, time, delta_t, T_max));

    end % while time march

    % Display time and bone temperature values of interest
    % (used for plotting externally)

    disp(sprintf('\nTime in seconds'));
    t_storage

    disp(sprintf('Temperature in Kelvin'));
    T_storage

end % main program

%% Functions

%%
function T = initial_conditions(ni,nj,z_in,r_in)

    T = zeros(ni,nj);

    for i = 1:ni
        for j = 1:nj

            z = z_in(i,j);
            r = r_in(i,j);

            % Units of cm have been converted to m for the domains of the
stem
            % cement and bone
```

```
            %% Stem
            if z >= 0.015 && z < 0.15
                if r >= 0.0 && r^2 <= ((1.0/100.0)^2)*(z-(3.0/200.0))
                    T(i,j) = 295.0;
                end
            end

            %% Cement
            if z >= 0.01 && z < 0.015
                if r >= 0.0 && r^2 <= ((1.0/50.0)^2)*(z-(1.0/100.0))
                    T(i,j) = 295.0;
                end
            end

            if z >= 0.015 && z < 0.15
                if r^2 > ((1.0/100.0)^2)*(z-(3.0/200.0)) && r^2 <=
((1.0/50.0)^2)*(z-(1.0/100.0))
                    T(i,j) = 295.0;
                end
            end

            %% Bone
            if z >= 0.0 && z < 0.01
                T(i,j) = 310.0;
            end

            if z >= 0.01 && z < 0.15
                if r^2 > ((1.0/50.0)^2)*(z-(1.0/100.0)) && r <= 0.0125
                    T(i,j) = 310.0;
                end
            end

            %% Body tissue to the right of the implant
            if z >= 0.15 && z <= 0.1625
                T(i,j) = 310.0; % Tissue temp. assumed to bone temp.
            end

        end
    end

end
%%
function alpha = maximum(a_s,a_c,a_b)
    if a_s > a_c && a_s > a_b
        alpha = a_s;
    elseif a_c > a_s && a_c > a_b
        alpha = a_c;
    else
        alpha = a_b;
    end
end
%%
function a = get_thermal_diffusivity(z,r,a_s,a_c,a_b)
```

```
    % Units of cm have been converted to m for the domains of the stem
    % cement and bone

    %% Stem
    if z >= 0.015 && z < 0.15
        if r >= 0.0 && r^2 <= ((1.0/100.0)^2)*(z-(3.0/200.0))
            a = a_s;
        end
    end

    %% Cement
    if z >= 0.01 && z < 0.015
        if r >= 0.0 && r^2 <= ((1.0/50.0)^2)*(z-(1.0/100.0))
            a = a_c;
        end
    end

    if z >= 0.015 && z < 0.15
        if r^2 > ((1.0/100.0)^2)*(z-(3.0/200.0)) && r^2 <= ((1.0/50.0)^2)*(z-
(1.0/100.0))
            a = a_c;
        end
    end

    %% Bone
    if z >= 0.0 && z < 0.01
        a = a_b;
    end

    if z >= 0.01 && z < 0.15
        if r^2 > ((1.0/50.0)^2)*(z-(1.0/100.0)) && r <= 0.0125
            a = a_b;
        end
    end

    %% Body tissue to the right of the implant
    if z >= 0.15 && z <= 0.1625
        a = a_b; % Body tissue assumed to have same therm. diff. as bone
    end

end
%%
function S = get_heat_source(z,r,S_in)

    % Units of cm have been converted to m for the cement domain

    %% Cement
    if z >= 0.01 && z < 0.015
        if r >= 0.0 && r^2 <= ((1.0/50.0)^2)*(z-(1.0/100.0))
            S = S_in;
        else
            S = 0;
        end
    end
```

```
    if z >= 0.015 && z < 0.15
        if r^2 > ((1.0/100.0)^2)*(z-(3.0/200.0)) && r^2 <= ((1.0/50.0)^2)*(z-
(1.0/100.0))
            S = S_in;
        else
            S = 0;
        end
    end

    %% Outside of cement domain
    if (z >= 0.0 && z < 0.01) || (z >= 0.15 && z <= 0.1625)
        S = 0;
    end

end
%%
function T_max = get_max_bone_temperature(ni,nj,z_in,r_in,T)

   T_max = 0.0;

   %% Bone and body tissue
   for i = 1:ni
       for j = 1:nj

           z = z_in(i,j);
           r = r_in(i,j);

           if (z >= 0.0 && z < 0.01) || (z >= 0.15 && z <= 0.1625)
               if T(i,j) > T_max
                   T_max = T(i,j);
               end
           end

           if z >= 0.01 && z < 0.15
               if r^2 > ((1.0/50.0)^2)*(z-(1.0/100.0)) && r <= 0.0125
                   if T(i,j) > T_max
                       T_max = T(i,j);
                   end
               end
           end

       end
   end

end
%%
function produce_plot(fig_num,z,r,T)
    figure(fig_num)
    contourf(z,r,T);
    title('Distribution of Temperature [K] in a Cement Femoral Implant');
    xlabel('z [m]');
    ylabel('r [m]');
    caxis([280 380]);
    colorbar;
end
```