JOURNAL OF THERMOPHYSICS AND HEAT TRANSFER
Vol. 22, No. 4, October–December 2008

Computer Simulation of Realistic Three-Dimensional Cemented Hip Arthroplasty: Thermal Osteonecrosis Analysis

Mauricio A. Sanchez*
IMTEC Corporation, Ardmore, Oklahoma 73401
Wagdy Rizk†
Beaumont Bone and Joint Institute, Beaumont, Texas 77707
Carlos A. Sanchez‡
Riskmetrics, Inc., Norman, Oklahoma 73071
and
Robert E. Cooper§
Western Autonomous University, Cali, Valle, Colombia

DOI: 10.2514/1.29157

Many current bone cements have proprietary minor ingredients that affect the chemical kinetics and heat transfer modeling of the exothermic reaction during bone cement polymerization. The geometry and the method of cooling or curing the bone cement can vary by application. We applied a complete numerical model using finite volume methods to investigate temperature history and thermal osteonecrosis analysis during and after bone cement polymerization for a commercial femoral component used in hip arthroplasty. Using a phenomenological kinetic model for energy generation, during bone cement exothermic reaction the effects of precooling and preheating parts of the femoral component before implantation were simulated. Numerical evidence shows that the temperature distribution along the bone depends upon the position of the stem with respect to the exterior bone boundary. Additionally, by precooling the stem, thermal osteonecrosis can be reduced in the bone through evidence of a thermal necrotic plane map of bone. Preheating the stem to above body temperature produces minimal thermal damage of the bone due to limited exposure time.

Nomenclature

A_o	=	constant, $1/\mathrm{s}$, Eq. (4)
C_p	=	specific heat, J/kg K
E	=	activation energy, J/mol
E_a	=	activation energy, J/mol, Eq. (4)
K_o	=	preexponential constant, $1/\mathrm{s}$
m	=	reaction order constant, Eq. (1)
n	=	reaction order constant, Eq. (1)
q	=	heat flux, $\mathrm{W/m^2}$
q_R	=	heat of reaction, $\mathrm{W/m^2}$
R	=	universal gas constant
$\dot{S}_c$	=	source term, $\mathrm{W/m^3}$, Eq. (2)
T	=	absolute temperature, K
t	=	time, s
x	=	position along bone, m
α	=	degree of reaction
$\kappa(T)$	=	Arrhenius equation, Eq. (4)
ρ	=	density, $\mathrm{kg/m^3}$
$\Omega(x)$	=	injury–severity–thermal–damage factor

Subscripts

b	=	bone
c	=	cement
s	=	stem

Received 4 December 2006; revision received 27 February 2008; accepted for publication 27 February 2008.

*Product Liaison Engineer, 2401 North Commerce Street. Member AIAA.
†Orthopedist, 3650 Laurel Avenue.
‡Software Developer, 2600 John Saxon Boulevard.
§Assistant Professor, Mechanical and Energy Department, 2 Vía Cali-Jamundí.

I. Introduction

POLYMETHYLMETHACRYLATE (PMMA) is an acrylic material composed of a powdered bone cement copolymer mixed with a monomer liquid methylmethacrylate [1] and is primarily used as an implant in many surgical specialties for joint replacement or augmentation and as a spacer; however, PMMA also has a number of short- and long-term effects connected with its use, one being an exothermic reaction which induces heat generation [2] in the bone cement during the curing process. This reaction may cause thermal osteonecrosis at the cement–bone interface, often considered the weak point of cemented arthroplasty, as well as polymer shrinking and void formation [3–6]. A number of clinical studies [7] have shown that cemented prostheses fail to function properly due to implant loosening and fatigue failure after long-term use.

So as to improve the strength of the interface, the cement requires deep interdigitation with the bone and low surface porosity while simultaneously avoiding the thermal osteonecrosis created by the heat generation source. After mixing the components of the PMMA, heat generation reaction occurs within 5 to 15 min, depending upon the cooling method (boundary conditions). This reaction generates excess heat with a peak temperature nearing 393 K. When applied to the implant, this high heat is capable of producing thermal necrosis in the bone tissue surrounding the cement, which limits the antibiotics that can be mixed to heat stable antibiotics, thus weakening the strength of the arthroplasty [8]. There are few available cooling modes for reducing peak temperature, yet one way is to reduce the rate of polymerization [9], which allows the heat to be released slowly; however, complete polymerization might not be fully attained. Another way for reducing the temperature of the cement while it polymerizes is to reduce the peak temperature. Experimentation [8] has shown that cooling the cement or stem leads to longer setting times and increases the risk of loosening, due to movement among the prosthesis, the cement, and the bone during the setting period, as well as the risk of void formation. To prevent void formation and improve the fatigue behavior of the cement, consideration has been given to preheating the femoral stem before implantation [4]; however, this might increase the chance of thermal osteonecrosis at the cement–bone interface. Clearly, when a large amount of heat is released due to polymerization, the temperature at the cement–bone interface is elevated. In addition to these temperature peaks, attention must be given to the exposure time to these high temperatures. Previous research has found that the temperature threshold for thermal injury is between 318 and 333 K [10], depending of course on the exposure time. Thus, the magnitude of the temperature and exposure time at the cement–bone interface are extremely important for maintaining the level of quality of the interface and the overall hip arthroplasty.

The main benefit of the research effort presented here is that it uses the realistic, fully three-dimensional (3-D) geometry of a femoral component used in total hip arthroplasty (THA). This project also expands on previous research in the use of PMMA for joint replacement, bone augmentation, and antibiotic spacers in orthopedic surgery. The numerical algorithm that couples the chemical kinetic model of the bone cement with the energy equation is also highly accurate and computationally efficient. Overall, simulation results offer significantly more definitive answers in the heat transfer modeling for several case scenarios used in THA. By using realistic values for thermophysical properties along with boundary and initial conditions throughout these numerical simulations, we evaluated the effects of the initial temperatures related to THA on system polymerization, temperature history, probability of thermal osteonecrosis, and the overall success of hip replacement. Also, in order to evaluate the probability of thermal damage, a damage factor was selected from appropriate literature [10] and was calculated based on transient temperature damage threshold levels.

II. Heat Transfer Model

To determine heat transmission and transient temperature behavior in the prosthesis–cement–bone system of a THA, a thermal analysis using a computational fluid dynamics (CFD) package (FLUENT) was performed. Previous thermal studies [2,4,6,8,11,12] have focused only on the corpus femoris (diaphysis) of the femur assuming a one-dimensional axisymmetric model. However, this part of the femoral component is not completely cylindrical, and the position of the stem relative to the exterior wall of the femur is of great importance to temperature distribution and osteonecrosis determination. Therefore, with the aim being to optimize the thermal analysis in cemented arthroplasties, the THA considered in this study was based on using (for the first time) a realistic geometric reproduction of an Endurance Total Hip System¶ as shown in Fig. 1a [13]. The model (Fig. 1b) consisted of a metallic prosthesis surrounded by, on average, a 3-mm-thick mantle of cement that was in turn embedded in the bone. Femur dimensions were modified** to fit those of an 82-year-old female cadaver located at the Funeral Service Department of the University of Central Oklahoma.††

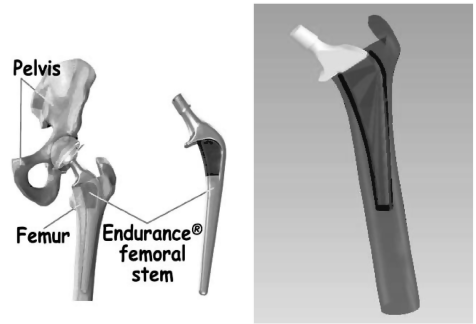
During curing, exothermic polymerization reaction induces heat generation in the bone cement, and to predict temperature distribution along the entire assembly and the degree of conversion in the cement as a function of the setting time during nonisothermal polymerization, an appropriate thermochemical model must be coupled with the heat conduction equation[2]. In this report, the cure polymerization kinetics of the bone cement were modeled by [4,11]

$$\frac{\partial \alpha}{\partial t} = K_o e^{(-E/RT)} \alpha^m (1-\alpha)^n \tag{1}$$

¶Endurance Total Hip System made by DePuy, a Johnson & Johnson Company. Some materials and instruments are identified in this report. In no instance does such identification imply recommendation.

**Computer-aided design (CAD) drawing of the femur was obtained from The Gustilo Medical Education Center headquartered in Minneapolis, MN.

††Funeral Service Department, Coyner Health Sciences Building, 100 University Boulevard, Edmond, OK 73034.



a) b)

Fig. 1 a) Rendering of the endurance femoral system [14]. b) Approximate prosthesis-cement-bone system.

where K_o is a preexponential constant, E is the activation energy, R is the universal gas constant, T is the absolute temperature, α is the degree of the reaction, and m and n are the reaction order constants. The degree of the reaction during curing ranges between zero and one. When there is no reaction, $\alpha = 0$; whereas $\alpha = 1$ indicates that no residual monomer (liquid) remains in the polymer [4].

To obtain the desired temperature distribution along the assembly, the following heat equation provides the basic tools for heat conduction analysis. The equation is given by [14]

$$\nabla \cdot q = -\frac{\partial}{\partial t} \rho C_p T + \sum \dot{S}_c \tag{2}$$

with

$$\dot{S}_c = \rho_c q_R \frac{\partial \alpha}{\partial t} \tag{3}$$

Equation (3) is the volumetric source term representing the cure polymerization kinetics of the bone cement with q_R as the heat of reaction. Equations (2) and (3) are solved using control volume discretization for the prosthesis, bone, and cement.

The bone cement modeled in this study is based on the experimental findings of Li et al. [4]. The experimental measurements of temperature distribution presented by Sanchez et al. [8] have good agreement with predictions using Eqs. (1–3) and the parameters $K_o = 5.206 \times 10^9 (1/\mathrm{s})$, $E = 67,891 \mathrm{J/mol}$, $m = 1.05$, $n = 1.10$, and $q = 125 \mathrm{kJ/kg}$, even though the bone cement (Simplex P, Howmedica, Inc.) is different than in [4]. Equation (3) is subjected to initial conditions at $\mathrm{t} = 0$ of $\alpha_o = 1.02 \times 10^{-4}$.

The initial amount of reacted monomer in the liquid component of the cement was represented in [4]. The exterior boundary condition of the system assumed that the bone had a constant body temperature of 310 K at the outer wall.

Because the solution of Eq. (2) was through continuous iteration, the calculations were performed via a step-by-step process in which the source term was calculated using a user-defined scalar (UDS) function inside FLUENT. Comparisons for the energy equation and the kinetic equation between current and previous iterations were made until convergence agreement was less than 1×10^{-6} before moving to the next time step. For this reason, the differential equation for the kinetic reaction Eq. (1) was solved using the Runge–Kutta–Feldberg method [15]. The effectiveness of this solution method was established by using a number of test problems from which the results were compared with those of the solver ODE15S provided by MATLAB and those of the partial differential equation coefficient form of COMSOL Multiphysics.

A. Threshold Level for Osteonecrosis

Bone cement has been used in orthopedic surgery (total joint arthroplasty and neurosurgery for cranial skeleton repair [16]) and to address various systemic or local patient complications. One of the most clinically important complications when using PMMA is thermal osteonecrosis around the bone–cement interface [16]. A number of reasons for thermal necrosis have been discussed in the literature, such as a local cytotoxic effect of the cement monomer, volumetric heat generation due to polymerization, and mechanical irritation of bone cells [4,12,16–24].

Temperature threshold levels for heat-induced tissue injury are time dependent [18]. Moritz and Henriques [19] report that cell necrosis for porcine and human skin occurs at a temperature of 328 K for 30 s of exposure; they also developed a burned injury damaged function which has been used extensively in documented literature [20]. Similar work by Lundskog [21] reports the effects of temperature on bone tissue and induced cellular necrosis at temperatures close to 323 K for periods greater than 30 s. Because exothermic reaction in the bone cement generates heat during polymerization, Sanchez et al. [8] recorded a temperature of 393 K at the center of a 2.54 cm sphere of cement; they also report temperatures up to 353 K at the surface of the spheres when cooled at room temperature. Obviously, this is sufficient heat to cause osteonecrosis and the generation of radiolucent zones following a cemented THA [22].

Numerical simulations of thermal bone necrosis have also been previously reported. Swenson and Schurman [23] demonstrate that the area of bone necrosis was dependent upon the width of the cement layer via using a simulation with 5- and 10-mm-width cement layers in THA. Mazzullo et al. [26] constructed a THA model with a 3-mm-wide cement layer around the stem and showed a 1.8-mm-wide bone necrosis area. However, most simulation models are based on outdated experimental work; thus, the criterion of thermal osteonecrosis is based solely on these previously developed theories.

Following the work by Moritz and Henriques [19], the corresponding thermal injury factor at any point in the tissue is given by solving Eq. (4) using the transient temperature distribution at a fixed point:

$$\Omega(x) = A_o \int \kappa(T)\,\mathrm{d}t \tag{4}$$

with $A_o = 8.0103 \times 10^{62}$ (1/s) and $\kappa(T)$ as an Arrhenius relationship with an activation energy value of $E_a = 4.05 \times 10^5$ (J/mol) which is considered to be temperature independent. The parameter $\Omega(x)$ represents the injury severity with respect to position x (meters), whereas $\Omega(x) = 0.53$ and $\Omega(x) = 1.0$ indicate visible burn injury and burn osteonecrosis [4,10,20], respectively.

B. Thermal Analysis

To determine the heat transmission and transient temperature behavior within the three-dimensional representation of the arthroplasty, a thermal analysis using a CFD package (FLUENT) was performed. The thermal and physical properties of the bone, bone cement, and prosthesis (cobalt chrome alloy) were assumed to remain constant during the entire heat transfer process. We assumed an initial body temperature of 310 K for the bone and a cement layer (mantle) of 3 mm for our simulation and then analyzed heat conduction. To investigate the feasibility of controlling temperature rise, we set different initial temperature conditions for the remaining system components (stem and bone cement) of the arthroplasty. The effects of precooling and preheating are similar to the ones used by Li et al. [4], which helped to validate the numerical computations obtained by the CFD code. Also, the effect of nonsymmetrical or irregular boundaries were included, which was not taken into account by Li and his fellow researchers.

III. Sensitivity Analysis and Results

To study the temperature development of the arthroplasty zone in the control volume model, we analyzed the temperature behavior in several horizontal planes covering the diaphysis and metaphysis sections of the femur as shown in Fig. 2. Plane 1 is located at the trailing edge of the stem where most of the analysis reported in the literature has been done while assuming one-dimensional cylindrical geometry. All planes (1–5) show that the stem is neither concentric along the femoral component nor is it cylindrical. Therefore, the geometrical position will have an influence on temperature distribution along the bone.

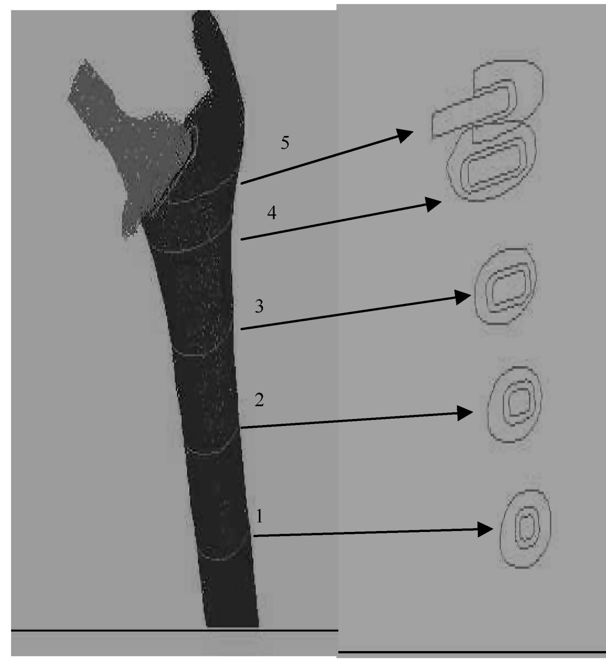


Fig. 2 Schematic comparing the plane areas for temperature development and necrotic mapping analyses.

As mentioned earlier, exothermic reaction induces heat generation in the bone cement during curing; a numerical analysis is done using a control volume approach through FLUENT. These equations are valid with the assumption that the mean density, heat capacity, and thermal conductivity of bone cement are used with no variation with respect to temperature and/or degree of reaction. It has been shown that the heat capacity of the composite C_p is dependent upon the temperature [6]. This property is treated as a constant, due to overshooting in the numerical model. C_p was defined by using the values in [8], and while reproducing the effects, it was verified that a very high rate of generated heat, coupled with thermal conductivity, is required to obtain a temperature increase in the cement. Thus, peak temperature is achieved when a balance occurs between the heat of reaction and conductivity.

In these simulations, the initial bone temperature was assumed to be 310 K, and all precooling and preheating were done by setting different initial temperatures for the remaining components of the THA. Precooling was achieved by setting the initial temperatures of the metallic stem and bone cement within a range between 278 and 296 K [4]. The same procedure was applied for the preheating process, where initial temperatures ranged from 296 to 318 K. Figure 3 shows the temperature–time history at one location (cement–bone interface) for the four different planes throughout the femur in four different cases. These histories were chosen because each had the highest peak temperature during the PMMA polymerization process. In case A, the temperature of the stem and cement was set to 296 K, whereas in cases B, C, and D, initial temperatures of the stem and cement were precooled to cement only at 278 K, stem only at 278 K, and both stem and cement at 278 K, respectively (see Table 1).

Table 1 Initial temperatures (K) for different simulation scenarios

	A	B	C	D	E	F
Bone	310	310	310	310	310	310
Cement	296	278	296	278	296	296
Stem	296	296	278	278	308	318

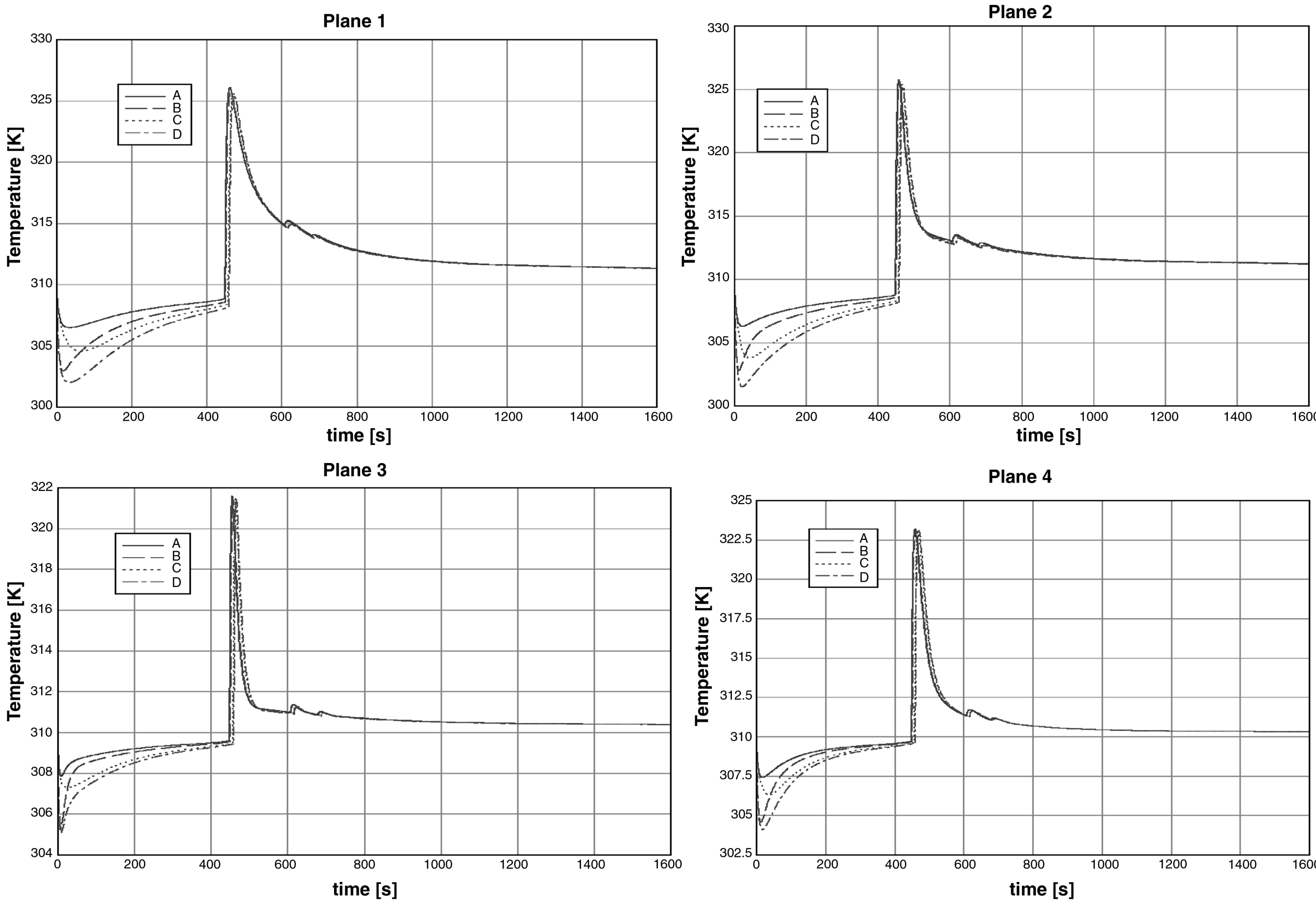


Fig. 3 Transient temperature distribution at the cement–bone interface for four different planes in the precooling procedure.

The results in Fig. 3 indicate that cement polymerization is rapid and delivers about 95% of its energy between 450 and 500 s for all four cases. This is somewhat different from previous one-dimensional simulations in which temperature delays are due to cooling effects [4,8,10,20]. However, it is assumed that this is only due to radial temperature distribution. In the three-dimensional case, the femur bulk affects and constant temperature ensures faster thermal equilibrium within all components of the THA. The peak constituent temperature occurred at the base of the prosthesis (Fig. 3, plane 1) with the cement–bone interface reaching 326 K, which agrees with the results of Swenson and Schurman [23]. Finally, Fig. 3 demonstrates that the decline in temperature after polymerization is faster for positions where the stem is not concentric with the femur shaft (see planes 2–4).

During the precooling procedures (cases B–D), the peak temperature at the cement–bone interface did not decrease substantially as expected and as reported in past literature [4,11]. As explained in the preceding paragraphs, sufficient thermal mass from the bone provides heat to the stem and cement. There is, of course, a small time delay linked to rapid exothermic reaction (lumped temperature increment) for the cooling cases in comparison to the ambient conditions reported in case A. This delay leads to a decrease in the thermal damage factor (Fig. 4) for the different chosen planes. Overall, these results suggest that, by cooling the stem and/or bone cement before implantation, the likelihood of thermal necrosis is substantially reduced [4]. These numerical predictions also suggest a small increment in setting time while cooling to 278 K (case D). However, there are few cooling modes to reduce the peak temperature. One way would be to reduce the rate of polymerization [9], thus causing the heat to be released slowly. Yet complete polymerization might not be fully attained, due to the absence of a peak temperature. Also, lowering the temperature of the cement while it polymerizes is another way to reduce peak temperature. Previous experiments [8] have shown that cooling the cement with saline leads to longer setting times and increases the risk of loosening, due to movement among the prosthesis, the cement, and the bone during setting periods.

During the preheating procedure, the metallic stem possesses an initial temperature greater than the body temperature; thus, preheating allows for better setting time of the THA. The objective of this numerical analysis was to obtain transient temperature distribution and a necrotic map along the femur for two different initial temperatures. For both initial stem temperatures (308 K–case E and 318 K–case F), the exothermic reaction occurred faster (85 s earlier) than case A or normal conditions (see Fig. 5). However, the peak temperature for the different planes was statistically identical for the cases previously studied. This time, the stem is the heat source while the cement and femur act as large sink sources. On the other hand, the necrotic map of Fig. 6 shows that there is visible thermal injury at the bottom of the stem. At the same time, when the bone thickness is larger (depending upon the side of the plane), the behavior is similar to plane 1. Therefore, preheating the stem at a temperature greater than the body temperature increases the likelihood of thermal osteonecrosis 0.5–1.0 mm beyond the cement–bone interface.

IV. Discussion

PMMA is one of the most commonly used alloplastic implants in hip arthroplasties and other orthopedic procedures and has the advantage of being very biocompatible and malleable because it rapidly polymerizes to become as hard as natural bone. Unfortunately, in hip arthroplasties, this polymerization process is also its greatest disadvantage [16] because during the hardening process, the temperature of the cement–bone interface reaches values up to 20° above body temperature for a period of time longer than 900 s. The temperature range needed to reach thermal cell osteonecrosis has been established to be between 321 and 343 K [24].

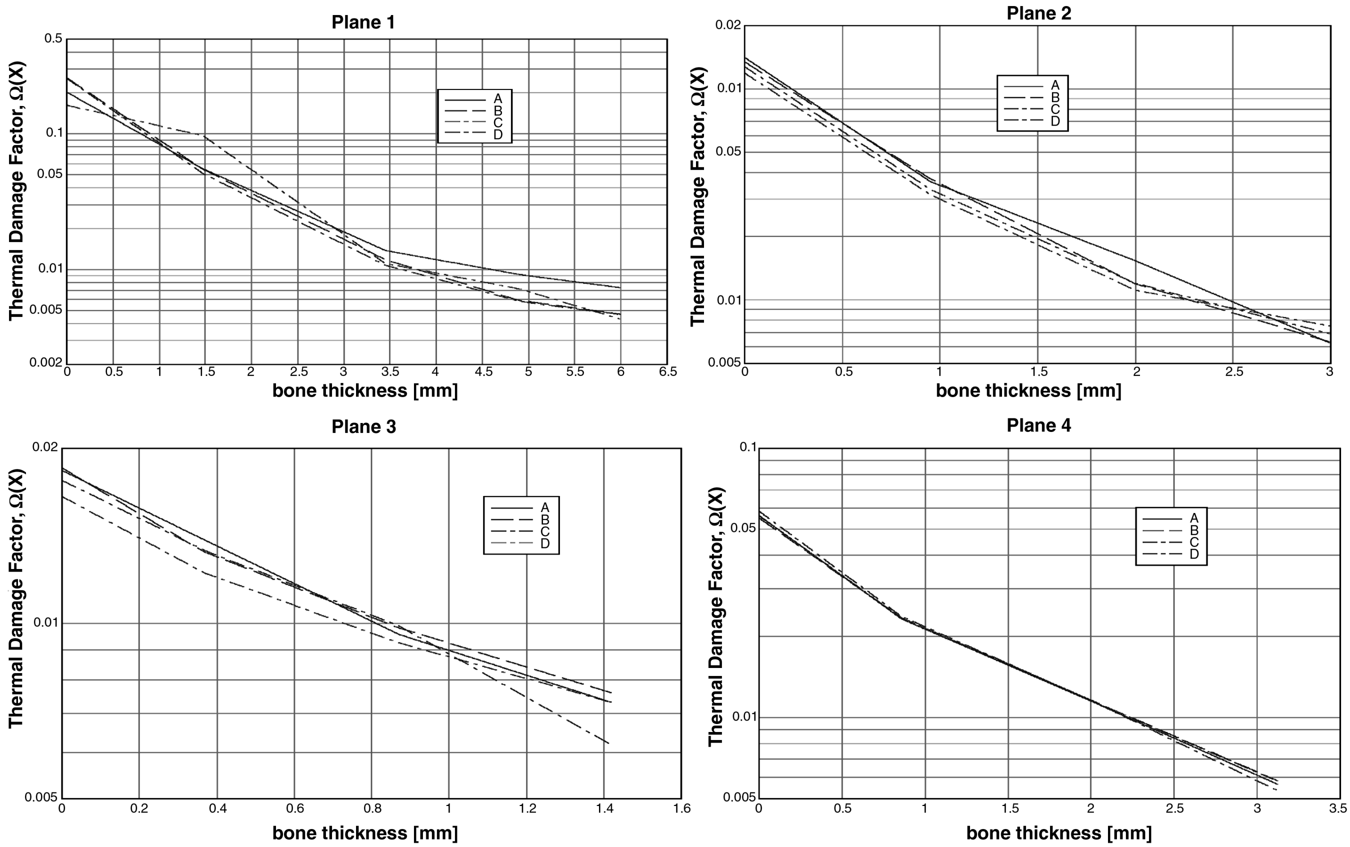


Fig. 4 Thermal damage factor (femoral necrotic map) on four different planes in the precooling procedure.

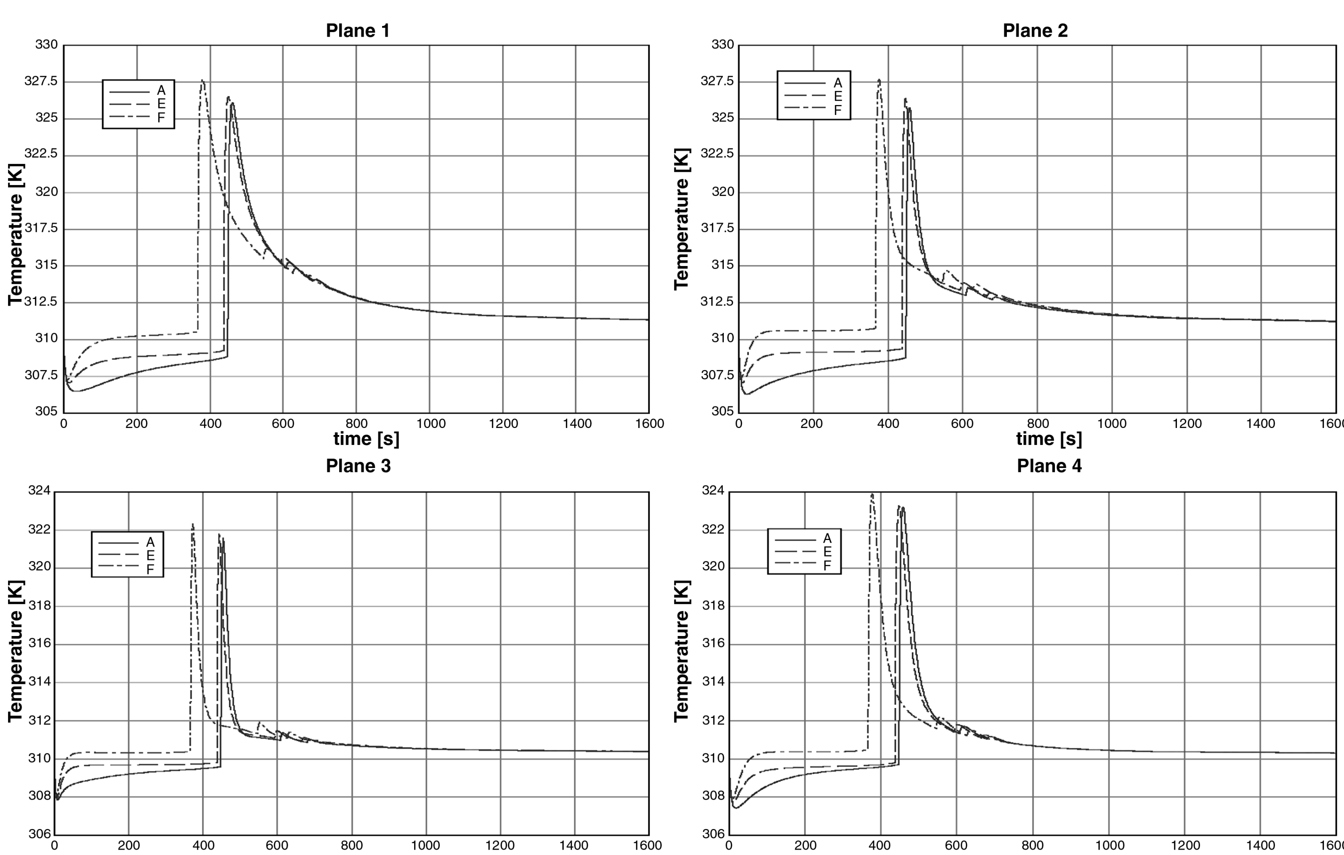


Fig. 5 Transient temperature distribution at the cement–bone interface on four different planes in the preheating procedure.

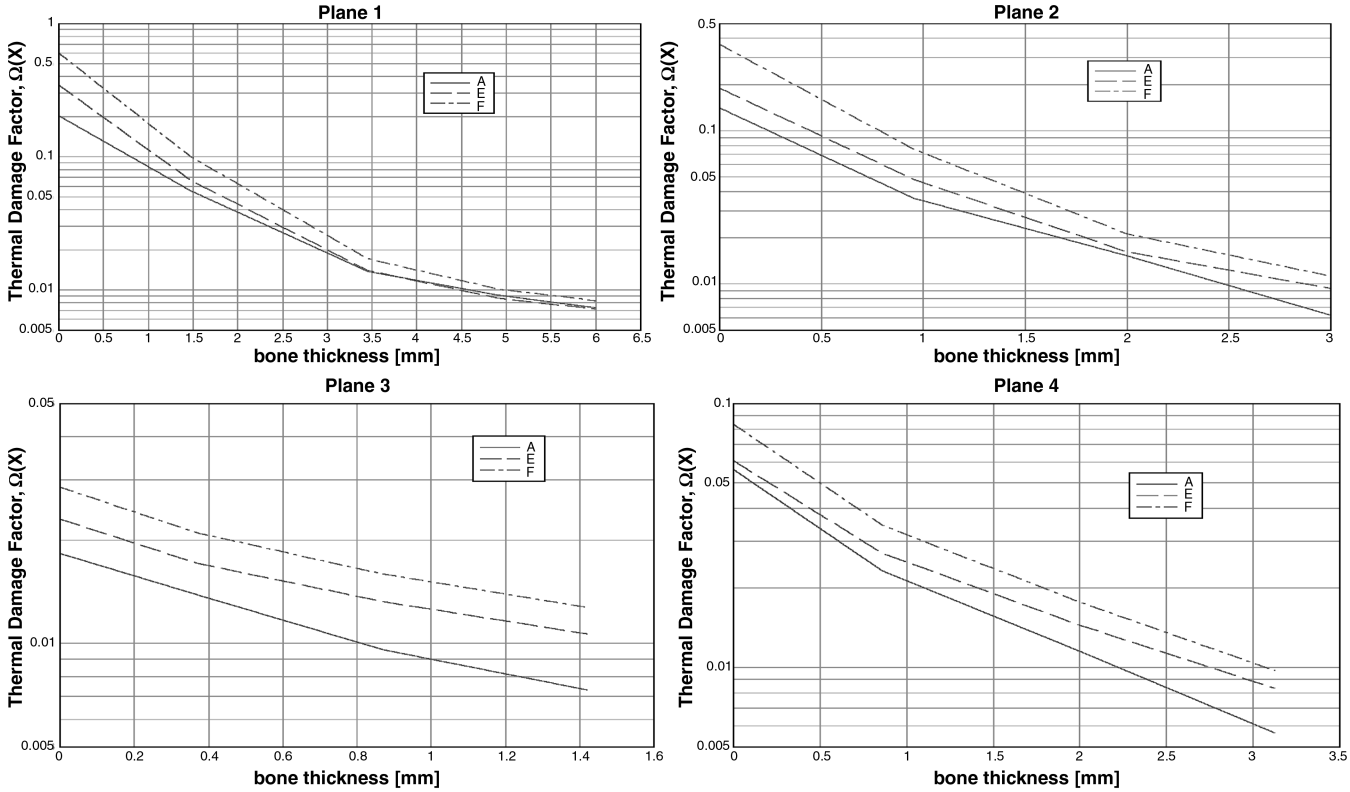


Fig. 6 Thermal damage factor (femoral necrotic map) on four different planes in the preheating procedure.

Concurrently, depending on the peak temperature reached, the time to cause cell death also varies. The results presented in this work and in [4,12,17,19,24] point out the temperature dependence inherent in thermal osteonecrosis criteria. For example, the temperature of 343 K is believed to kill cells instantly, and 323 K needs to be maintained up to 30 s to produce cell death [25]. For our results, cell death temperature range could be reached in most common, self-curing acrylic cement implants at the cement–bone interface and many cell layers deep into the bone.

Previous numerical simulations of thermal bone necrosis by Swenson and Schurman [23] showed that the area of bone necrosis was due to the width of the cement layer by a simulation with 5- and 10-mm-wide cement layers in THA [23]. Huiskes [17] constructed a necrotic map of THA which showed that the temperature of the cement layer around a cup was more than 373 K and that there was about a 2-mm width of bone necrosis area and about 2-mm width of vascular damage area external to the necrosis. Mazzullo et al. [26] constructed a THA model with a 3-mm-wide cement layer around the stem which showed a 1.8-mm width of bone necrosis area.

Over the years, several methods have been used to lessen heat injury to the bone during polymerization [8], such as reducing the amount of cement thickness; precooling the implant, the cement, and/or the bone with saline irrigation; and reducing the polymerization rate. In this numerical simulation, we show a 1-mm width of bone necrosis with a 3-mm-thick cement layer in the THA model; thus, the thinner the cement layer, the smaller the bone necrotic area. Indeed, a thinner cement layer may be better for thermal bone necrosis, but correspondingly worse for the strength of the cement fixation. There is a tradeoff on what is considered the best option between preventing necrosis and compromising the strength of the THA. In essence, it is recommended that the cement layer be less than 3 mm in width to prevent thermal necrosis and to gain enough strength for the THA.

Previous studies [12] have reported that as the temperature of the bone tissue increases (due to the heat released by the exothermic reaction), the thermal damage factor $\Omega(x)$ also increases. As the bone tissue temperature reaches its physiological value, $\Omega(x)$ reaches a constant value which is demonstrated for planes 2–4, where there is not enough bone space for heat to propagate. As such, the thermal necrosis factor is lower at that particular position. These results indicate that the volume of the cement and the femur itself play important roles in temperature distribution and thermal osteonecrosis of the bone. A comparison of the results from the three-dimensional simulations in the present work with corresponding one-dimensional simulations demonstrates that temperature distribution is comparable between the two simulations. However, the magnitude of the rebound (the thermal damage factor) predicted by one-dimensional is larger as compared with that of the three-dimensional simulation. Our results suggest that the one-dimensional simulation may be sufficient for the computation of the temperature field with cemented THA design and development so that different configurations can be analyzed and an optimal design chosen before further prototype development and detailed experimental evaluation is undertaken. However, for detailed heat injury in the vicinity of the bone–cement interface, a three-dimensional simulation is necessary.

During the preheating procedure, it was established that the likelihood of thermal damage increases as the initial temperature of the stem is also increased. However, the residual stress after polymerization was shown to decrease [4] at the stem–cement interface. Concurrently, more osteolysis is produced at the cement–bone interface, thus increasing the fatigue failure at this interface. However, as pointed out by Li et al., [4], early fatigue failure appears to be less critical at the cement–bone interface, where changes occur due to biological factors rather than dynamic factors, yet the advantages of the preheating procedure clearly surpass the contradictory effects in cemented THA.

These numerical predictions were based on a control volume formulation using a very fine tetrahedral grid which increases the computational time but allows more accurate answers at the femoral region and others of importance; thus, the influence of thermal contact resistance at the cement–bone interface on the thermal damage was very low. Also, experiments performed on the 82-year-old femur showed a similar temperature distribution at this interface, and the results were comparable to the numerical simulations. It should also be pointed out that the effect of the bioheat equation might have an impact on temperature history and thermal osteonecrosis determination.

In vivo studies found the maximum temperatures at the bone–cement interface range from 313 to 321 K [27] in 3-mm-thick cement. Other in vitro studies found the maximum temperature to range from 309 to 326 K, depending on the mixing technique. Finally, empirical models [27] (usually one-dimensional) have predicted a maximum temperature at the bone–cement interface in 3-mm-thick cement region to lie between 308 to 316 K at the diaphysis section. Hence, this realistic model agrees very well with both the in vivo and in vitro studies.

The thermal damage factor is greater at the diaphysis section of the femur than in the metaphysis. However, it is not comparable to the one-dimensional simulations published in previous documents [4]. For this particular THA model, the damage factor was low at the methaphysis section because all heat is dissipated to the stem in lieu of the short duration of higher temperatures. However, for other types of THA configurations where more bone surrounds the stem, the thermal damage factor can be of great importance in the analysis of cemented hip arthroplasties.

The temperature in bone cement also affects the use of antibiotics. For instance, antibiotics are mixed with the bone cement during prophylaxis in arthroplasty, the treatment of infected arthroplasty, the treatment of oesteomyelitis, and the treatment of open fractures [8]. It has long been a common belief within the orthopedic community that only aminoglycosides can be mixed with bone cement because they are heat stable [9], and it is clear that other specific antibiotics are heat liable and, therefore, are rendered biologically inactive by the heat emitted during the polymerization process of bone cement. A literature review shows [28] that chloramphenicol and tetracycline appear to be the only antibiotics that become inactivated when mixed with bone cement, whereas other studies [23] have investigated the bioactivity of different antibiotics after being mixed with bone cement. It has been shown [29,30] that gentamicin, tobramycin, and vancomycin are stable in PMMA and diffuse from the cement in active form. Therefore, this numerical investigation supports the idea that different antibiotics (e.g., cephalosporins, quinolones, and penicillins) when mixed with PMMA remain biologically active. Certainly, precooling procedures increase the likelihood of antibiotic efficacy in THA.

Presently, bone cement consists mainly of PMMA, but at this time, new cements are being developed that, overall, exhibit much lower curing temperatures than PMMA. For instance, researchers have clinically tested bioactive bone cement in which the highest surface temperature is around 308 K [8]. Biodegradable bone cements have a maximum crosslinking temperature between 311 and 321 K, which is much lower than the crosslinking temperature of 367 K for PMMA cement [18]. It is expected that these new cements will have practical uses in preventing thermal bone necrosis as a result of polymerization.

The most straightforward method to avoid thermal osteonecrosis is to refrain from using cemented implants at all, in favor of the cementless versions. There are, however, extensive clinical data from postoperative follow-ups indicating that the percentage of failures is significantly lower in cases of cemented prostheses. Also, cementless implants are avoided in the case of weaker bones, for example in rheumatoid patients [25]. Therefore, this realistic analysis is needed and can work as a validation tool in the continuous development of cement-based THAs.

V. Conclusions

To investigate the feasibility of controlling temperatures and the likelihood of thermal osteonecrosis, numerical simulations were conducted to determine the temperature and necrotic map in a commercial THA. Under these conditions, peak temperatures were established and exposure time was determined with the aim to demonstrate heat reaction progress along the femur. Results have shown that bone cement thickness and size definitely have an effect on peak temperature. In humans, peak temperatures could be detrimental to any surrounding tissue; thus, maintaining low-boundary temperatures results in an exothermic reaction that lowers the temperature and allows less osteonecrosis and better antibiotic mixing. However, this also holds the chance of increasing setting time during the polymerization process. Because a higher temperature peak is achieved due to poor heat dissipation along the cement–bone interface, this might translate into bone necrosis, especially in preheating procedures.

In modern operating rooms, two specific methods are used related to know when the cement is cured. When the cement is used as an implant, the polymerization occurs during mostly dry conditions. Contrary to this, when cement is used as a spacer, curing occurs during wet conditions, due to the presence of irrigation solution and body fluids. Thus, these numerical simulations demonstrate temperature history in THA implants and indicate that minimal thermal damage when preheating the stem and that mechanical behavior might improve due to less setting time.

The discrepancies between the results from one-dimensional calculations to three-dimensional calculations are clearly due to the three-dimensional nature of the problem. As a consequence, any attempt to interpolate between a series of parallel one-dimensional sections to reconstruct an equivalent three dimensional volume is likely to produce errors in physical parameter estimates for this particular case. Therefore, we have concluded that three-dimensional implementation of the quantitative thermal damage factor determination compensation provides the best necrotic map in terms of quantitative accuracy, spatial resolution, and noise at a cost of high computational requirements.

Acknowledgments

This publication was made possible by grant number P20RR016478-04 from the National Center for Research Resources (NCRR), a component of the National Institutes of Health (NIH). The authors thank Derrick Strickland and Joseph A. Grzybowski for their immense collaboration.

References

[1] Wininger, D. A., and Fass, R. J., "Antibiotic-Impregnated Cement and Beads for Orthopedic Infections," *Antimicrobial Agents and Chemotherapy*, Vol. 40, No. 12, 1996, pp. 2675–2679.

[2] Borzacchiello, A., Ambrosio, L., Nicolais, L., Harper, E. J., Tanner, K. E., and Bonfield, W., "Isothermal and Non-Isothermal Polymerization of a New Bone Cement," *Journal of Materials Science: Materials in Medicine*, Vol. 9, No. 6, 1998, pp. 317–324. doi:10.1023/A:1008898712929.

[3] Woo, L., Loos, A. C., and Springer, G. S., "Heat of Reaction, Degree of Cure, and Viscosity of Hercules 3501-6 Resin," *Journal of Composite Materials*, Vol. 16, No. 6, 1982, pp. 510–521. doi:10.1177/002199838201600605

[4] Li, C., Schmid, S., and Mason, J., "Effects of Pre-Cooling and Pre-Heating Procedures on Cement Polymerization and Thermal Osteonecrosis in Cemented Hip Replacements," *Medical Engineering and Physics*, Vol. 25, No. 7, 2003, pp. 559–564. doi:10.1016/S1350-4533(03)00054-7

[5] James, S. P., Schmalrized, T. P., McGarry, F. J., and Harris, W. H., "Extensive Porosity at the Cement-Femoral Prosthesis Interface: A Preliminary Study," *Journal of Biomedical Materials Research*, Vol. 27, No. 1, 1993, pp. 71–78. doi:10.1002/jbm.820270110

[6] Nzihou, A., Sharrock, P., and Ricard, A., "Reaction Kinetics and Heat Transfer Studies in Thermoset Resins," *Chemical Engineering Journal*, Vol. 72, No. 1, 1999, pp. 53–61. doi:10.1016/S1385-8947(98)00137-5

[7] Hung, J-P., Chen, J-H., Chiang, H-L, and Wu, J. S-S., "Computer Simulations on Fatigue Behavior of Cemented Hip Prostheses: A Physiological Model," *Computer Methods and Programs in Biomedicine*, Vol. 76, No. 2, 2004, pp. 103–113. doi:10.1016/j.cmpb.2004.05.004

[8] Sanchez, M. A., Sutton, W. H., Rizk, W., and Tompkins, J., "Thermal Curing and Strength of PMMA Bone Cement," Heat Transfer Conference, Las Vegas, American Society of Mechanical Engineers, Paper HT2003-47067, July 2003.

[9] Goodell, J. A., Flick, A. B., Hebert, J. C., and Howe, J. G., "Preparation and Release Characteristics of Tobramycin-Impregnated Polymethylmethacrylate Beads," *American Journal of Hospital Pharmacy*, Vol. 43, 1986, pp. 1444–1460.

[10] Li, C., Kotha, S., Huang, C-H., Mason, J., Yakimicki, D., and Hawkins, M., "Finite Element Thermal Analysis of Bone Cement for Joint Replacement," *Journal of Biomedical Engineering*, Vol. 125, No. 3, 2003, pp. 315–322.

[11] Maffezzoli, A., Ronca, D., Guida, G., Pochini, I., and Nicolais, L., "In-Situ Polymerization Behavior of Bone Cements," *Journal of Materials Science: Materials in Medicine*, Vol. 8, No. 2, 1997, pp. 75–83. doi:10.1023/A:1018502731892

[12] Li, C., Khota, S., and Mason, J., "Evaluation of the Effects of Implant Materials and Designs on Thermal Necrosis of Bone in Cemented Hip Arthroplasty," *Bio-Medical Materials and Engineering*, Vol. 13, No. 4, 2003, pp. 419–428.

[13] Joint replacement information at http://www.jointreplacement.com/ [cited 24 Feb. 2006].

[14] Kaviany, M., *Principles of Heat Transfer*, Wiley-Interscience, New York, 2002, Chap. 2, p. 79.

[15] Lee, H. J., and Schiesser, W. E., *Ordinary and Partial Differential Equation Routines in C, C++, Fortran, Java, Maple, and Matlab*, CRC Press, Boca Raton, FL, 2003, Chap. 5.

[16] Stelnicki, E. J., and Ousterhout, D. K., "Prevention of Thermal Tissue Injury Induced by the Application of Polymethylmethacrylate to Calvarium," *Journal of Craniofacial Surgery*, Vol. 7, No. 3, 1996, pp. 192–195. doi:10.1097/00001665-199605000-00006

[17] Huiskes, R., "Heat-Generation and Conduction Analyses of Acrylic Bone Cement in Situ," *Acta Orthopedica Scandinava. Supplementum*, Vol. 185, 1980, pp. 43–108.

[18] Fukushima, H., Hashimoto, Y., Yoshiya, S., Kurosaka, M., Matsuda, M., and Kawamura, S., "Conduction Analysis of Cement Interface Temperature in Total Knee Arthroplasty," *Kobe Journal of Medical Sciences*, Vol. 48, 2002, pp. 63–72.

[19] Moritz, A. R., and Henriques, F. C., Jr., "Studies on Thermal Injury II. The Relative Importance of Time and Surface Temperature in the Causation of Cutaneous Burns," *The American Journal of Pathology*, Vol. 23, 1947, pp. 695–720.

[20] Diller, K., and Hayes, L., "A Finite Element Model of Burn Injury in Blood-Perfused Skin," *Journal of Biomechanical Engineering*, Vol. 105, No. 3, 1983, pp. 300–307.

[21] Lundskog, J., "Heat and Bone Tissue. An Experimental Investigation of the Thermal Properties of Bone Tissue and Threshold Levels for Thermal Injury," *Scandinavian Journal of Plastic and Reconstructive Surgery*, Vol. 9, 1972, pp. 1–80.

[22] Mjoberg, B., Pettersson, H., Rosenqvist, R., and Rydholm, A., "Bone Cement, Thermal Injury and the Radiolucent Zone," *Acta Orthopaedica Scandinavica*, Vol. 55, No. 6, 1984, pp. 597–600.

[23] Swenson, L. W., Jr., and Schurman, D. J., "Finite Element Temperature Analysis of a Total Hip Replacement and Measurement of PMMA Curing Temperature," *Journal of Biomedical Materials Research*, Vol. 15, No. 1, 1981, pp. 83–96. doi:10.1002/jbm.820150112

[24] Nelson, C., Krishnan, E., and Neff, J., "Consideration of Physical Parameters to Predict Thermal Necrosis in Acrylic Cement Implants at the Site of Giant Cell Tumors," *Medical Physics*, Vol. 13, No. 4, 1986, pp. 462–488. doi:10.1118/1.595852

[25] Stanczyk, M., and Telega, J. J., "Heat Transfer Problems in Orthopaedics," *Engineering Transactions*, Vol. 51, 2003, pp. 267–306.

[26] Mazzullo, S., Paolini, M., and Verdi, C., "Numerical Simulation of Thermal Bone Necrosis During Cementation of Femoral Prosthesis," *Journal of Mathematical Biology*, Vol. 29, No. 5, 1991, pp. 475–494. doi:10.1007/BF00160473

[27] Hansen, E., "Modeling Heat Transfer in a Bone-Cement-Prosthesis System," *Journal of Biomechanics*, Vol. 36, No. 6, 2003, pp. 787–795. doi:10.1016/S0021-9290(03)00012-5

[28] Arciola, C. R., Campocciaa, D., and Montanaro, L., "Effects on Antibiotic Resistance of Staphylococcus Epidermidis Following Adhesion to Polymethylmethacrylate and to Silicone Surfaces," *Biomaterials*, Vol. 23, No. 6, 2002, pp. 1495–1502. doi:10.1016/S0142-9612(01)00275-7

[29] Lundberg, A., and Hedlund, H., "Antibiotic Bone Cement as a Prophylactic Means in Joint Replacement Surgery," *Infection and Local Treatment in Orthopedic Surgery*, edited by E. Meani, C. Romanò, L. Crosby, G. Hofmann, and G. Calonego, Springer-Verlag, New York, Pt. 2, 2007.

[30] Masri, B. A, Duncan, C. P., and Beauchamp, C. P., "Long-Term Elution of Antibiotics from Bone-Cement: An in Vivo Study Using the Prosthesis of Antibiotic-Loaded Acrylic Cement (PROSTALAC) System," *Journal of Arthroplasty*, Vol. 13, No. 3, 1998, pp. 331–338. doi:10.1016/S0883-5403(98)90179-6