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Theoretical Simulation of Temperature Elevations in a Joint Wear Simulator During Rotations

The objective of this study is to develop a theoretical model to simulate temperature fields in a joint simulator for various bearing conditions using finite element analyses. The frictional heat generation rate at the interface between a moving pin and a stationary base is modeled as a boundary heat source. Both the heat source and the pin are rotating on the base. We are able to conduct a theoretical study to show the feasibility of using the COMSOL software package to simulate heat transfer in a domain with moving components and a moving boundary source term. The finite element model for temperature changes agrees in general trends with experimental data. Heat conduction occurs primarily in the highly conductive base component, and high temperature elevation is confined to the vicinity of the interface in the pin. Thirty rotations of a polyethylene pin on a cobalt-chrome base for 60 s generate more than 2.26 °C in the temperature elevation from its initial temperature of 25 °C at the interface in a baseline model with a rotation frequency of 0.5 Hz. A higher heat generation rate is the direct result of a faster rotation frequency associated with intensity of exercise, and it results in doubling the temperature elevations when the frequency is increased by 100%. Temperature elevations of more than 7.5 °C occur at the interface when the friction force is tripled from that in the baseline model. The theoretical modeling approach developed in this study can be used in the future to test different materials, different material compositions, and different heat generation rates at the interface under various body and environmental conditions. [DOI: 10.1115/1.4026158]

Keywords: bioheat transfer, joint simulator, temperature elevations, simulation

Introduction

Total joint replacement has relieved millions of arthritic patients of constant pain and decreased function, dramatically improving their lives, and remains the most effective treatment for arthritis. The most common bearing couple used for total joint replacements is ultra-high molecular weight polyethylene (UHMWPE) polymer (as the tibial component of an artificial knee, or the acetabular/pelvic component of an artificial hip),

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articulating against a cobalt-chromium (CoCr) metal alloy. The metal is harder and more wear resistant than the UHMWPE, and therefore, the polymer is gradually damaged by wear. UHMWPE hip components wear at a rate of 100–300 $\mu\text{m}/\text{year}$ [1], generating trillions of polymer particles with a size range of 0.1–1 μm [2]. Particles in this size range are believed to be the instigators of a cascade of biological events that eventually results in osteolysis or bone resorption [3]. Osteolysis can lead to loosening of the implanted device components and results in a vicious cycle of increased wear and further osteolysis, pain, or even fracture of the device due to cyclic and impact loading. In many cases, costly revision surgery is required to alleviate the pain and loss of function.

Recent improvements in the wear resistance properties of UHMWPE through crosslinking and antioxidant additives show promise in delaying osteolysis [4], though there are still long-term concerns of particle generation and fatigue fracture. Alternatives to the UHMWPE-CoCr bearing couple include metal-on-metal (MoM), ceramic-on-ceramic, ceramic-on-carbon fiber reinforced polyether ether ketone (CFR-PEEK), and other combinations of bearing couple materials, but there are limitations to each of these. The low fracture toughness of ceramics has resulted in catastrophic fracture [5]. Loss of tissue, bone, muscle, and nerves has resulted from metal wear particles and ions generated by wear of MoM total joint replacements, causing immobility for life in some patients [6]. CFR-PEEK is a new material with virtually no clinical history. As artificial joint technology has matured, total joint replacement has been used in younger and more active patients who require an even longer lasting implant that, at the same time, must be even more wear resistant [7]. The total joint bearing couple used for these more active patients may be expected to see greater loads and a higher relative velocity between opposing wear surfaces, and the more demanding biomechanical environment may lead to greater wear as well as higher friction-generated temperature rises at the implant and in the surrounding fluids.

The heat generated by friction between different hip joint replacement bearing couples has been measured clinically. Implant temperatures measured in telemetrized hip prostheses, after one hour of walking, were reported to be around 43 $^{\circ}\text{C}$ [8] and about 46 $^{\circ}\text{C}$ in the synovia [9]. Intracapsular percutaneous temperatures from sensors implanted in both hip joints after walking on a treadmill 3–4 km/hour for 60 min were reported in Ref. [10]. For the nine different implants used, the temperature increases varied from 3 $^{\circ}\text{C}$ to 8 $^{\circ}\text{C}$. The temperatures of hip joint replacements have also been measured in bench tests under simulated clinical wear conditions using a hip simulator. The equilibrium temperatures of the lubricant (bovine serum is the most commonly accepted lubricant for simulating joint fluid) for UHMWPE acetabular cups bearing against alumina, CoCr, and diamond-like carbon in a hip simulator were reported as 33, 36, and 34 $^{\circ}\text{C}$, respectively, in a room temperature environment [11]. In another hip simulator study of UHMWPE acetabular cups bearing against zirconia, CoCr, and alumina balls at room temperature, steady state (equilibrium) temperatures of the lubricant was 38.2, 35.8, and 33.2 $^{\circ}\text{C}$, while the maximum subsurface temperatures of the UHMWPE were 51, 40.4, and 35.6 $^{\circ}\text{C}$ [12].

In total joint replacements, where one or both of the opposing articulating components are made of materials that have a low thermal conductivity (e.g., PEEK's thermal conductivity is 64 times lower than CoCr and half that of UHMWPE), temperature elevations due to frictional heat are expected to be higher. For example, in a joint simulator study using a pin-on-disk (PoD) machine (in which wear of a joint bearing couple is simulated by rubbing a pin made of one of the bearing couple materials against a disk made of the other), PE on PEEK bearing couples were reported to have a higher friction and higher temperatures than PE on CoCr bearing couples [13]. Temperature increases in joint simulators are of concern because as less heat is conducted away from the wear surface, the temperature of the lubricant is elevated, and proteins in the lubricant become denatured [14], forming

unnatural solid particles, a process that does not occur in vivo. These denatured particles artificially protect the bearing surfaces from wear and ultimately lead to artificially low wear [15]. For this reason, temperature control has been suggested as one way to better simulate implant wear [16,17].

The orthopedic industry is currently very active in evaluating various bearing materials for the future by conducting laboratory simulated wear testing. Joint simulators, in which wear of the actual prosthesis is tested, have had some success in modeling wear prior to clinical use [18], though wear rates in these simulators are often lower than those generated in vivo. This is attributed to phenomena that increase wear clinically but are unaccounted for in the joint simulators [19–22]. Clinical wear is affected by various factors, including materials, prosthetic design, surgical technique, and patient parameters. Wear mechanisms of new materials and the effect of friction and temperature can be studied by using PoD wear simulator devices without complicating design geometry effects of joint prostheses. PoD devices are simple, inexpensive, and provide reliable wear test measurements for screening prosthetic joint materials if a clinically relevant “cross-shear” wear path pattern is used [23]. Computational finite element methods have been used to study maximum contact pressure and heat generation during hip simulation [24,25]. One computer model study predicted temperatures within a hip joint wear simulator on the cup surface, head surface, and bath [26], including a peak temperature of 51 $^{\circ}\text{C}$ at the contact surface and a 3 $^{\circ}\text{C}$ temperature gradient through the thickness of the cup.

The objective of this study was to evaluate the temperature field in a PoD joint simulator for different bearing couple materials using numerical simulation. Frictional heat was mostly dissipated through the metal base. The technical challenge in this study is how to implement a moving calculation domain (the pin) in finite element methods using a commercial software package. Therefore, it can realistically simulate the temperature fields during rotations of the pin on the base. Data from these types of theoretical studies can be used to determine the maximum temperature elevation in simulators and the dominant factors that contribute to the temperature elevations, as well as to identify temperature monitoring sites.

Methods

A numerical model was developed based on the geometry of an example joint simulator for evaluating long term wear behavior. The simulator consists of three major components: a flat base representing the cup in a realistic joint, a cylinder representing the joint ball, and a thin lubricant layer between the base and the cylinder (Fig. 1(a)). Note that the cylinder is held and controlled

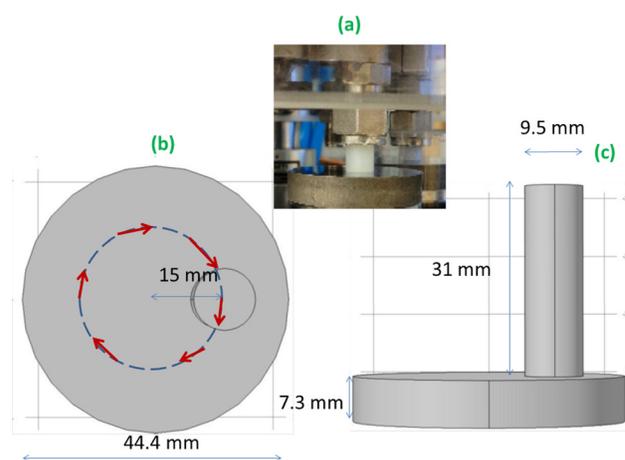


Fig. 1 The experimental setup of the joint simulator and the computer modeling of the pin and the base: (a) experimental setup, (b) top view of the computer model, and (c) side view of the computer model

to rotate on the base at a specific frequency. The load exerted on the cylinder is also controlled to represent the realistic load in a clinical settings.

Our numerical model was developed using the COMSOL 4.3 software package (COMSOL, Inc., Burlington, MA) (Fig. 1(b) top view, Fig. 1(c) side view). The base is represented by a cobalt-chrome disk with a diameter of 44.4 mm and thickness of 7.3 mm. The cylindrical pin is made of ultra-high molecular weight polyethylene and is 9.5 mm in diameter and 31 mm long. The lubricant layer is typically very thin, approximately only several micrometers, which would present difficulty in creating the mesh in simulation. The lubricant layer was, therefore, not explicitly included in our model; however, it was included implicitly by the heat generation rate due to friction, and was modeled as a boundary heat source at the interface between the pin and the base. The pin rotates around the base center with a center-to-center distance of 15 mm. The governing equation for either the base or the pin is the traditional heat conduction equation

$$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T \quad (1)$$

where ρ is density, c is specific heat, k is thermal conductivity, and T is temperature. No heat generation occurs inside either the base or the pin. Instead, the heat generation rate due to friction is modeled as a boundary heat source at the interface. Heat generation at the interface may be due to fluid friction and dynamic friction with lubricant. Preliminary calculations have demonstrated that the fluid friction force is several orders of magnitude smaller than the dynamic friction force. Therefore, the contribution from fluid friction is neglected in this study. The heat generation rate ($Q_{\text{generation}}$) due to dynamic friction is calculated by the following equation:

$$Q_{\text{generation}} (\text{J/s}) = \text{friction coefficient} * \text{load} * \text{velocity} \quad (2)$$

where the velocity at the center of the pin is calculated from the frequency of the rotation and the center-to-center distance. The calculated $Q_{\text{generation}}$ is the interface heat source used in the model. Since the pin rotates, the interface heat source also moves with the pin. The bottom surface of the base and the top surface of the pin are prescribed as adiabatic boundary conditions while the side surfaces of the base and the pin are subject to a combined convection and radiation boundary condition (overall heat transfer coefficient $h = 10 \text{ W/m}^2 \text{ }^\circ\text{C}$, $T_\infty = 25 \text{ }^\circ\text{C}$) [27,28]. The top surface of the base is exposed to ambient environment of $25 \text{ }^\circ\text{C}$. Heat convection occurs from this surface to the surrounding air, and evaporation cooling from the lubricant layer to a relatively dry air environment cannot be neglected. Although the lubricant layer is not explicitly included in our model as a physical layer, evaporative cooling due to presence of the lubricant is accounted for in this study. The combined thermal effect of convection and evaporation is incorporated into the boundary condition at this surface as

$$-k \frac{\partial T}{\partial n} \Big|_s = h(T - T_\infty) + q''_{\text{evaporation}} \quad (3)$$

where h is again the overall heat transfer coefficient, k is the thermal conductivity of the base, and n is the normal direction of the top surface of the base. The evaporative cooling heat flux ($q''_{\text{evaporation}}$ in Eq. (3)) represents energy needed for water (lubricant) to change phase from liquid to vapor at a rate of 0.01 kg/ (hour m^2) [28], resulting in $q''_{\text{evaporation}}$ equal to 110 W/m^2 . The evaporation rate is estimated based on calculations of the mass transfer coefficient as $3.97 \times 10^{-3} \text{ m/s}$, determined from the average Sherwood number as 6.378 [28]. The humidity of the room is assumed as 70%. The initial condition of the simulation is $25 \text{ }^\circ\text{C}$ in the domain in equilibrium with the surroundings.

The differential equations for both components are solved using the finite element solver of COMSOL[®] Multiphysics 4.3. The mesh is refined in the vicinity of the interface. The total number of the tetrahedral elements using the fine mesh setting is 60,609. The mesh sensitivity is checked by increasing the mesh setting to extremely fine meshing with an increase in the total number of elements to 326,668. The five-fold increase in the number of mesh elements results in a difference of less than $0.1 \text{ }^\circ\text{C}$ in the resulting maximum temperature in the simulation domain.

Results and Discussion

Table 1 gives the thermal properties of the base and the pin [12,14]. The baseline model consists of a friction coefficient of 0.065 obtained from a previous study [12], a load of 354 N, and a rotation frequency of 0.5 Hz. Using the parameters in the baseline model, the rotation velocity is 0.047 m/s under the rotation frequency of 0.5 Hz, and the total heat generation rate at the interface is then calculated as 1.08 W. The total heat generation rates at the interface for various combinations of the load, the friction coefficient, and the rotation frequency are shown in Table 2. The data show that the heat generation rate at the interface is proportional to the frequency, the load, or the friction coefficient. Specifically, doubling the load will result in the same heat generation rate at the interface as if the friction coefficient is doubled.

Simulations are performed over a total of 60 s due to limitations of computer memory and other resources. The COMSOL software allows the pin to move along the circular path following a specific rotation velocity while the heat generation rate source at the interface is also moving at the same rotation speed as the pin. The resulting temperature contours in the three-dimensional simulation domain can be seen in Fig. 2, where the four images give the different pin locations on the base component within one rotation. It clearly shows that the COMSOL software is capable of modeling a moving component. This figure demonstrates a continuous temperature elevation at the interface between the base and the pin and continuous heat conduction to the rest of the base region. In contrast, most of the pin region shows almost no temperature elevations.

Figure 3 presents the temperature contours in the side view of the baseline model. The first image shows the initial uniform temperature field of $25 \text{ }^\circ\text{C}$. The second image gives the temperature field after the fifth rotation ($t = 10 \text{ s}$, Fig. 3(b)), and the maximum temperature elevation at the interface is approximately $1.28 \text{ }^\circ\text{C}$; later, it continues to rise. Once the 25th rotation ($t = 50 \text{ s}$) is completed, the maximum temperature at the base is around $27.24 \text{ }^\circ\text{C}$, $2.24 \text{ }^\circ\text{C}$ higher than its initial temperature of $25 \text{ }^\circ\text{C}$ (Fig. 3(f)). The noncontinuous heat generation rate at the interface of any specific

Table 1 Thermal properties of the components

	k (W/m $^\circ\text{C}$)	ρ (kg/m 3)	c (J/kg $^\circ\text{C}$)
Base (cobalt-chrome)	14.86	8387	422.87
Pin (UHMWPE)	0.21	900	1000

Table 2 Simulation parameters of various cases

	Friction coefficient	Frequency (Hz)	Load (N)	Velocity (m/s)	$Q_{\text{generation}}$ (W)
Baseline	0.065	0.5	365	0.047	1.08
Effect of	0.065	1.0	365	0.094	2.16
Frequency	0.065	2.0	365	0.188	4.32
Effect of Load	0.065	0.5	730	0.047	2.16
	0.065	0.5	1095	0.047	3.24
Effect of Friction	0.130	0.5	365	0.047	2.16
Coefficient	0.195	0.5	365	0.047	3.24

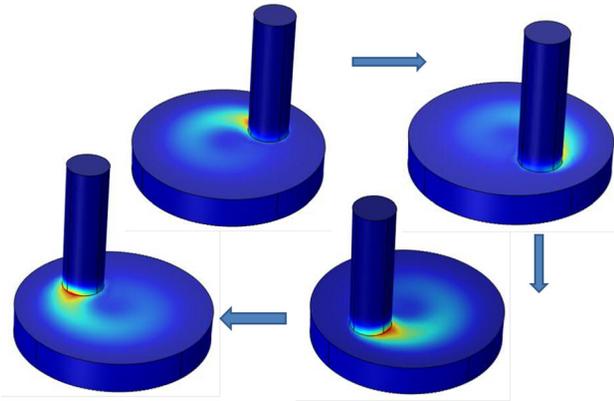


Fig. 2 The 3D images during the simulation of one rotation of the pin on the base. All images are taken from the same angle. Notice the movement of the pin on the base.

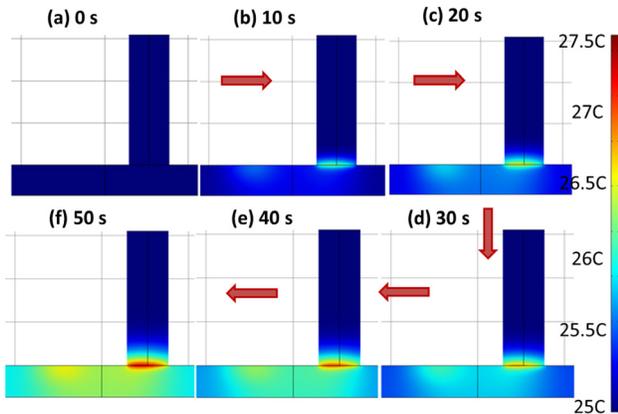


Fig. 3 Side view of the simulated temperature fields in the pin and the base at the initial condition (a), at end of the 5th (b), the 10th (c), 15th (d), 20th (e), and 25th (f) rotation

base region due to the rotation of the pin resulted in on-and-off patterns of the temperature behavior. However, due to the frequency of the rotation, one can still see significant residual heat remaining in the base component.

Temperature elevations in the base component are evident as the pin rotates (Fig. 4). Due to the friction-induced heat generation, a tail-like region of elevated temperature can be seen following the pin's track. Comparing Fig. 4(b) (after the fifth rotation) to Fig. 4(f) (after the 25th rotation), one can see significant heat accumulation in the base component. In addition, the maximum temperature observed in the top view does not occur exactly at the center of the pin's bottom surface, and there are large temperature variations at the interface (Fig. 4(f)). Therefore, it suggests that the location of a temperature sensor at the interface may greatly affect the recorded temperature value since it is not a uniform temperature field on the surface of the interface. For the top surface of the base not in direct contact with the pin, the temperature rises steadily to 25.7–26.5 °C after the 25th rotation. The steady increase in the base region of the disk not in direct contact with the pin is similar to an experimental observation of a lubricant temperature being 0.7 °C higher than its external environment in a previous study [29].

Since the temperature field on the surface of the interface is not uniform, one may average the temperature on the interface surface and use it to show how the temperature of the lubricant at the interface is elevated during rotations. Figure 5 illustrates the averaged interface temperature over time. It clearly shows a larger temperature jump at the first several rotations with a temperature

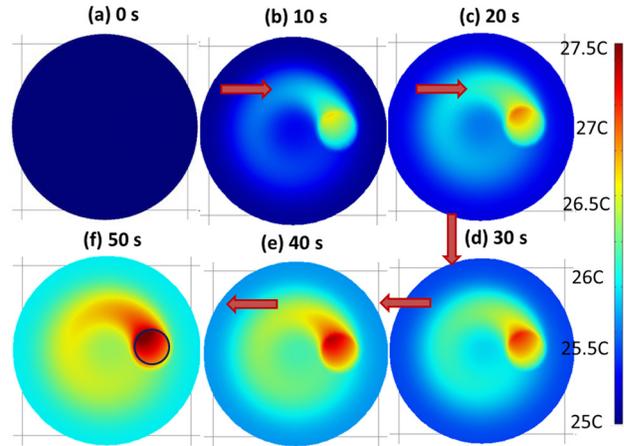


Fig. 4 Top view of the simulated temperature fields on the top surface of the base at the initial condition (a), at end of the 5th (b), the 10th (c), 15th (d), 20th (e), and 25th (f) rotation. The black circle in (f) represents the location of the interface between the pin and base.

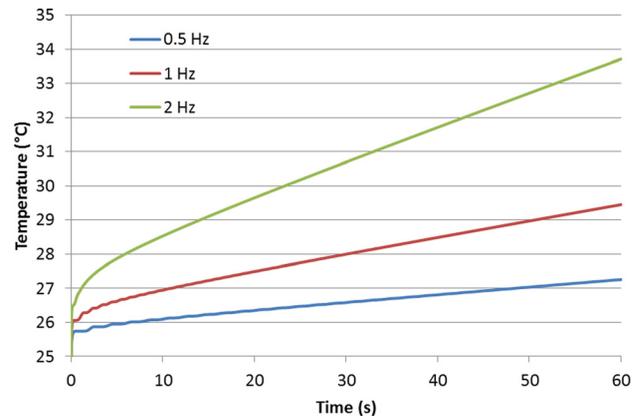


Fig. 5 Effect of the rotation frequency on the averaged temperature at the interface between the pin and the base

rise rate of 0.3898 °C/s after the first rotation in the baseline model. After that, heat conduction to the surrounding pin and the base materials occurs, and the rate of temperature rise decreases. The temperature rise rates are 0.0286 °C/s, 0.0242 °C/s, 0.023 °C/s, 0.0226 °C/s, 0.0224 °C/s, and 0.0222 °C/s, after the 5th, 10th, 15th, 20th, 25th, and 30th rotation, respectively. Based on the simulation results over 60 s, it is unlikely that the quasi-steady state will be established quickly. In fact, in previous experimental studies, temperatures at the interface between a joint and its socket continue to rise even after 420 min of rotations [12].

Rotation frequency is an important factor that affects the heat generation rate at the interface. An increase in the rotation frequency may be due to changes in intensity of motion, like exercise. As shown in Table 2, doubling the rotation frequency will result in the same work (Joule) per rotation; however, the heat generation per unit time is doubled. Figure 5 compares interface temperature rises under different rotation frequencies. After 60 s (30 cycles, 60 cycles, or 120 cycles for the three frequencies, respectively), temperature elevations at the interface from the initial 25 °C are 2.26 °C, 4.45 °C, and 8.72 °C, almost proportional to the rotation frequency (or the heat generation rate at the interface).

Friction force is determined by both the load and the friction coefficient. Variation of body weight may affect how much the joint will bear, varying from half of the body weight to approximately four times the body weight. The friction coefficient, on the

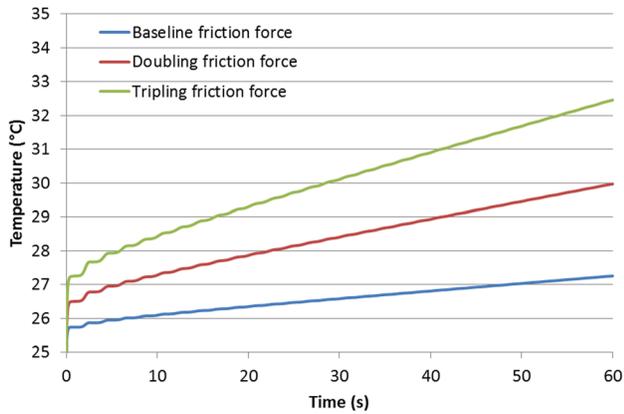


Fig. 6 Effect of the friction force on the averaged temperature at the interface between the pin and the base

other hand, will depend on the lubricant between the joint and its socket. In this study, we decouple the load from the friction coefficient and assume they may vary independently from each other. As shown in Eq. (2), doubling the load will result in the same heat generation rate at the interface as if the friction coefficient is doubled (Table 2); therefore, the resulting temperature elevations will be the same. Figure 6 demonstrates how the temperature elevations at the interface are affected by either the load or the friction coefficient by doubling or tripling the friction force (load \times friction coefficient) from the baseline simulation. Doubling the friction force increases the temperature elevation from 2.26 °C to 4.97 °C after the 30th cycle while tripling the friction force further results in a 7.46 °C increase from its initial temperatures. Again the temperature elevation rate seems proportional to the friction force.

One limitation of this study is the short simulation time of 60 s due to limited computational resources. Since there is a very large temperature gradient at the interface between the pin and the base, very fine meshes are needed there, adding to the computational requirements. Reasonable agreement is found with limited experimental measurements [29]; however, it is difficult to directly compare our results to previous experimental results by other groups because of differences in experimental setups, the thermal environment of the setup, and estimation of friction-generated heat generation rate at the interface. Nonetheless, our simulation results are consistent with previous measurements of temperature elevations at the interface during continuous rotations of the joint (pin). Previous studies have shown that the temperature elevations can be as low as 6 °C in vivo after 60 min [8] or as high as 31 °C in a simulator after 420 min of rotations [12]. Those are significant increase in temperature of the lubricant at the interface, and it is possible to induce thermal damage to the proteins in the lubricant. Therefore, lowering the friction force at the interface by developing better model lubricant is an important step to minimize thermal damage in those tissue regions. In addition, the poorly conductive material used in most artificial joints restricts the availability to conduct heat away from the interface. For example, the thermal conductivity of the UHMWPE pin used in this study is only 1/3 of that of tissue, which does not allow fast heat dissipation from the interface. One possible modification of the design is to use highly conductive materials with a specific coating on both the joint head and the socket to conduct heat away from the interface.

In summary, we were able to conduct a numerical study to show the feasibility of using the COMSOL software package to simulate heat transfer in a domain with moving components and a moving boundary source. The finite element model for temperature changes agrees in general trends with experimental data. Thirty rotations of a polyethylene pin on the cobalt-chrome generated more than a 2.26 °C temperature elevation from its initial

temperature of 25 °C in the baseline model, and the temperature elevations are proportional to the rotation frequency or the friction force. Mild temperature elevations occur primarily in the highly conductive base component, and high temperature elevation is confined to the vicinity of the interface in the poorly conductive pin. The numerical modeling can be used in the future to predict the behavior of different materials, material compositions, and heat generation rate at the interface under various body and environmental conditions to develop improved artificial joints.

Acknowledgment

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