Thermal analysis of bone cement polymerisation at the cement–bone interface

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Abstract

The two major problems that have been reported with the use of polymethylmethacrylate (PMMA) cement are thermal necrosis of surrounding bone due to the high heat generation during polymerisation and chemical necrosis due to unreacted monomer release. Computer models have been used to study the temperature and monomer distribution after cementation. In most of these models, however, polymerisation is modelled as temperature independent and cancellous bone is modelled as a continuum. Such models thus cannot account for the expected important role of the trabecular bone micro-structure. The aim of this study is to investigate the distribution of temperature and monomer leftover at the cancellous bone–cement interface during polymerisation for a realistic trabecular bone—cement micro-structure and realistic temperature-dependent polymerisation kinetics behaviour.

A 3-D computer model of a piece of bovine cancellous bone that underwent pressurization with bone–cement was generated using a micro-computed tomography scanner. This geometry was used as the basis for a finite element model and a temperature-dependent problem for bone cement polymerisation kinetics was solved to simulate the bone cement polymerisation process in the vicinity of the interface. The transient temperature field throughout the interface was calculated, along with the polymerisation fraction distribution in the cement domain.

The calculations revealed that the tips of the bone trabeculae that are embedded in the cement attain temperatures much higher than the average temperature of the bone volume. A small fraction of the bone (10%) is exposed to temperatures exceeding 70°C, but the exposure time to these high temperatures is limited to 50 s. In the region near the bone, the cement polymerisation fraction (about 84%) is less than that in the centre (where it is reaching values of over 96%). An important finding of this study thus is the fact that the bone tissue that is subjected to the highest temperatures is also subjected to high leftover monomer concentration. Furthermore the maximum bone temperature is reached relatively early, when monomer content in the neighbouring cement is still quite high.

Keywords: Bone cement; Polymerisation; Heat generation; Micro-CT; Finite element analysis

1. Introduction

Polymethylmethacrylate (PMMA) bone cement is widely used in orthopaedic surgery, mainly for fixation of prostheses but also for stabilizing compressive vertebral fractures or filling bone defects. The two major problems that have been reported with the use of this cement are thermal necrosis of surrounding bone due to the high heat generation during polymerisation (DiPisa et al., 1976; Feith, 1975; Homsky et al., 1972), and chemical necrosis due to unreacted monomer release (Feith, 1975; Linder, 1977; Albrektsson and Linder, 1984; Lu et al., 2002). Since the polymerisation kinetics, and thus the amount of monomer leftover, depends on the temperature, the temperature distribution during polymerisation is one of the most important determinants for the success of the cementation procedure.

The temperature of the bone surrounding the cement during polymerisation has been measured in vitro (e.g. Borzacchiello et al., 1998; Deramond et al., 1999; Fukushima et al., 2002; Dunne and Orr, 2002) and in vivo (e.g. Toksvig-Larsen et al., 1991). A problem with these studies, however, is the fact that the temperature can be measured at a limited number of
locations only. To overcome this problem, computer models based on the finite element method have been used for the calculation of the full 2-D or 3-D temperature profiles (Mazzullo et al., 1991; Baliga et al., 1992; Fukushima et al., 2002; Hansen, 2003). In these studies, however, cement and bone are usually modelled as homogenous continuum materials and the interface between them is modelled as infinitely thin and is characterized by its conductivity only. In particular, when cancellous bone is considered, such analyses are of limited value for three reasons. First, the thermal properties of bone tissue and marrow that together constitute the cancellous bone are not the same. The thermal properties of cancellous bone thus will depend on the bone volume fraction. Second, the bone–cement interface is not infinitely thin, but in fact represents a complex 3-D structure with cement penetrating in some of the voids, thus enclosing some of the trabeculae. Due to their relatively high conductivity, these penetrating trabeculae can provide an efficient heat sink. The temperature distribution near the interface thus largely depends on the interlock between cement and trabeculae. Third, although continuum models can provide temperature distributions in the homogenized material, they do not provide information about the temperature in cement, bone and void domains separately. Hence, these studies cannot quantify the temperature in the bone tissue itself, which, given the fact that bone cells are located in this tissue, seems the most relevant measure to study thermal necrosis. Consequently, in order to calculate more realistic temperature distributions in cement-cancellous bone constructs, more detailed models are required, that can account for the micro-structure of cancellous bone.

In an early study, Huiskes (1980) used a generic 2-D FE model of the bone–cement interface to investigate the thermal properties of the cancellous bone–cement interface. This model provided first information about the conductivity of the cancellous bone–cement interface and about the temperature distribution in the bone tissue itself. It was reported that the temperature in the trabeculae could be much higher (78°C) than in the neighbouring bone (50°C), demonstrating the importance of micro modelling for accurate estimation of the tissue temperature. Given its generic and 2-D geometry, however, it is not very clear how realistic this model is for the calculation of the temperature distribution. Also, in that study, the polymerisation was modelled as temperature independent and only the steady-state solution was reported. To the best of our knowledge, no later studies exist in which more sophisticated and 3-D models were used for the interface.

Realistic and 3-D models of an actual bone architecture at the level of the trabeculae can be generated nowadays with micro-computed tomography (micro-CT) reconstruction techniques. Modelling of time and temperature-dependent polymerisation is now possible with advanced finite element codes. The aim of this study therefore is to investigate the distribution of temperature and monomer leftover at the cancellous bone–cement interface during polymerisation for a realistic bone–cement architecture and realistic temperature-dependent polymerisation kinetics behaviour.

2. Methods

2.1. Temperature problem formulation

The temperature field resulting from the cement polymerisation is described by the usual Fourier–Kirchhoff equation (here we assume that the physical properties are independent of temperature)

$$\frac{\partial T(\mathbf{x}, t)}{\partial t} = a_i \nabla^2 T(\mathbf{x}, t) + q_i(\mathbf{x}, t) \quad \text{in } \Omega_i,$$

where

$$q_i(\mathbf{x}, t) = \eta(\mathbf{x}, t) \frac{Q}{\rho_1 c_1} \frac{\partial w(\mathbf{x}, t)}{\partial t}. \tag{2}$$

Here index \(i = 0,1,2\) denotes, respectively, bone, cement and marrow. The respective domains are denoted by \(\Omega_i\). \(T\) is the temperature, \(t\) denotes time, \(a_i\) is the thermal diffusivity, \(\rho_1\) and \(c_1\) stand for the density and specific heat of the cement, respectively, and \(Q\) is the latent heat generated by cement polymerisation. The function \(\eta(\mathbf{x})\) is defined as follows:

$$\eta(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega_1, \\ 0 & \text{otherwise.} \end{cases} \tag{3}$$

This formulation needs to be supplemented with an additional kinetic equation for the polymerisation fraction \(w\). Here the model due to Mazzullo et al. (1991) is adopted

$$\frac{\partial w(\mathbf{x}, t)}{\partial t} = a \exp \left( - \frac{E_a}{RT(\mathbf{x}, t)} \right) P(T(\mathbf{x}, t), w(\mathbf{x}, t)), \tag{4}$$

where \(a = 2.6397 \times 10^8 \text{ (1/s)}\) and \(E_a = 62866 \text{ (J/mol)}\) (Mazzullo et al., 1991) are model constants and \(R\) is the universal gas constant.

The function \(P(T, w)\) is defined in the following way:

$$P(T, w) = \begin{cases} \frac{2}{w^* (T)} w^{1-\frac{1}{2}} (w^* (T) - w)^{1+\frac{1}{2}} & \text{if } w < w^* (T), \\ 0 & \text{if } w \geq w^* (T). \end{cases} \tag{5}$$

Here \(z = 9.2\) is the model constant (cf. Mazzullo et al., 1991). The equilibrium polymerisation fraction \(w^*\) is
defined by

\[ w^* = \begin{cases} 
\frac{T}{T_g} & \text{if } T \leq T_g, \\
1 & \text{if } T > T_g,
\end{cases} \tag{6} \]

where \( T_g = 378 \text{ K} \) is the glass transition temperature.

Eqs. (1)–(6) comprise the formulation of the transient problem of polymerisation kinetics coupled to heat conduction. One also needs the boundary and initial conditions for the two field variables: the temperature \( T \) and the degree of polymerisation \( w \).

2.2. Specimen preparation and imaging

A cube (approx. 1 cm edge length) of bovine, trabecular bone, frozen to \(-20^\circ\text{C}\) was cut from the trochanteric region. The specimen was cleaned and the marrow near one side was removed with a brush after which the specimen was cleaned again. Cement used in this study was a mixture of two commercially available cements: Codman cranioplastic bone cement (Johnson&Johnson) and CMW1 radiopaque (DePuy Ltd.). The powder components of these cements were mixed in the ratio 1:1 and the cement was prepared by mixing this powder blend with the liquid component of the Codman cranioplastic bone cement. This procedure was developed in the course of several experiments in order to produce \( \mu \text{CT} \) images on which the cement could be uniquely identified. This was not possible with one of both cement types alone. The Codman cranioplastic is a non-radiopaque, slow-setting PMMA bone cement which is indistinguishable from marrow cavities on \( \mu \text{CT} \) images. On the other hand, CMW1 radiopaque is indistinguishable from bone. The mixing produced cement that would show an intermediate intensity on \( \mu \text{CT} \) images.

The cement was mixed and placed directly on the bone surface within a rubber ring. A load of ca. 150 N was applied to the top of the cement while it was curing (Fig. 1.).

After curing for 1 h at room temperature, the specimen was scanned in a micro-computer tomography (micro-CT) device (\( \mu \text{CT} 80 \), Scanco Medical). A total of 35 sequential images were made at a resolution of 50 \( \times \) 50 \( \mu \text{m} \) (Fig. 2.). The thickness of each slice was 50 \( \mu \text{m} \), such that a 3-D reconstruction was obtained that is built of isotropic voxels.

A 1.75 mm \( \times \) 1.75 mm \( \times \) 5.95 mm sub-volume with its longest edge perpendicular to the bone–cement interface was selected for further processing (35 \( \times \) 35 \( \times \) 119 cubic voxels having edge lengths of 0.05 mm). A modest Gaussian filtering procedure was used to reduce the noise in the images after which the domain was segmented using a two-level threshold procedure. With this approach, all voxels with a grey-value lower than the lower-threshold were identified as marrow, those with a grey-value between the lower and higher threshold were identified as cement, and those with a grey-value larger than the second threshold value were identified as bone. This procedure effectively separated the three materials. However, due to a partial-volume effect, voxels near the boundary of trabeculae also displayed grey-values less than the higher threshold. To avoid that cement properties would be assigned to such voxels, the 3-D contours of the cement area were determined and cement properties were assigned only to voxels within this area. The resulting model could then be visualised by assigning different colours to the bone, cement and marrow domains (Fig. 3.).

2.3. Finite element modelling

A special computer program was written to convert the 3-D reconstruction generated by the scanning software to an input file for the finite element code Abaqus (Abaqus 6.2, Hibbit, Karlsson & Sorensen) that was used for solving the transient temperature problem formulated in Eqs. (1)–(6). The final model consisted of
145,775 elements, of which 39,067 (ca. 27%) represented bone tissue, 42,362 (ca. 29%) cement and the remaining—bone marrow.

The following initial conditions were applied:

\[ T_{|t=0}(x) = 300 \text{ K}, \quad (7) \]

\[ w_{|t=0}(x) = 0.01. \quad (8) \]

The nonzero initial value for the polymerisation fraction is necessary for the initialisation of the polymerisation process (see Eqs. (4) and (5)). For small values of \( w_{|0} \), its exact value does not influence the final temperature or polymerisation fraction fields. It only affects the length of the initial “warm-up” period. Based on results of additional studies that were done to investigate the role of this parameter, a value \( w_{|0} = 1\% \) was chosen.

On all the walls perpendicular to the interface the adiabatic condition is adopted:

\[ \frac{\partial T}{\partial n} = 0. \quad (9) \]

This condition is also applied to the leftmost wall (Fig. 3). It is further assumed that this wall is positioned at the centre of the cement mantle such that the peak temperature is reached here. This reasoning gives the rationale for the adiabatic condition. On the rightmost wall (Fig. 3) the convection condition is imposed:

\[ \frac{\partial T}{\partial n} = h(T_0 - T), \quad (10) \]

where \( h = 5 \) (W/m²K) (value corresponding to free convection) and \( T_0 = 310 \) K. An overview of all thermal parameters used for the analyses is given in Table 1. The data were collected from Fukushima et al. (2002) and Starke et al. (1998). For marrow, water properties were assumed. Approximately 52 h of computer time were required for solving the resulting problem on a SGI Origin200 workstation computer.

<table>
<thead>
<tr>
<th></th>
<th>Density (kg/m³)</th>
<th>Thermal conductivity (W/mK)</th>
<th>Specific heat (J/kg/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>cement</td>
<td>1000³</td>
<td>0.17b</td>
<td>1600b</td>
</tr>
<tr>
<td>bone tissue</td>
<td>2000³</td>
<td>0.4a</td>
<td>1300b</td>
</tr>
<tr>
<td>marrow</td>
<td>1000</td>
<td>0.6</td>
<td>4190</td>
</tr>
</tbody>
</table>

Data after

\[^a^\text{Starke et al. (1998)}, \text{water properties were assumed for marrow.}\]^b\text{Fukushima et al. (2002).}\]

3. Results

The peak bone temperature was reached at \( t = 112 \) s (Fig. 4). It can be seen that the temperature in the bone/marrow region (307 K) is much less than the maximum values reached in the bone or cement (337 K).

The simulation ended at \( t = 300 \) s (Fig. 5). It is clearly visible that in the region near the bone, the cement polymerisation fraction (about 84%) is less than that in the centre (where it is reaching values of over 96%). After \( t = 300 \) s the polymerisation is virtually completed; no further changes in the polymerisation fraction take place and the specimen cools down slowly. It can be clearly seen (Fig. 6), that the polymerisation fraction rapidly increases between \( t = 70 \) and \( 100 \) s, at which time it has reached an average value of about 90%. The analysis of the polymerisation fraction as a function of the longitudinal coordinate and time (Fig. 7) shows that polymerisation at the centre of the cement occurs earlier and is more complete than that near the bone interface.

The fraction of bone volume exposed to a temperature exceeding one of 6 chosen levels: 45°C, 50°C, 55°C, 60°C, 65°C and 70°C seems the most relevant measure to assess bone cell survival (Fig. 8). It can be seen, for example, that all of the bone is exposed to a temperature higher than 45°C starting from \( t = 140 \) s until the end of...
the analysis \((t = 300)\). Only a small fraction of the bone (10%), however, is exposed to temperatures exceeding 70°C, and the exposure time to these high temperatures is limited to 50 s \((t = 75\) until 125).

4. Discussion

According to the presented results, tips of the bone trabeculae extending deep into cement are exposed, for short duration, to temperatures in excess of 70°C and are in a prolonged contact with the volume of cement containing substantial monomer leftover (more than 15%, - Fig. 5). Differences in temperature throughout the cement mantle are up to 20 K and differences in the polymerisation fraction reach up to 12.6%. Such inhomogeneities are not described by temperature-independent models of polymerisation available in literature (see Jefferis et al., 1975; Huiskes, 1980; Swenson Jr. et al., 1981). To grasp them one
needs more elaborate models, such as presented by Mazzullo et al. (1991) (used in the present study), Baliga et al. (1992), Hansen (2003) or Stańczyk (submitted).

It was found in this study that temperatures in the bone-marrow region adjacent to the bone–cement interface were much lower than those in the cement-embedded trabeculae. Neglecting the bone–cement interpenetration, as is done in earlier studies that modelled the bone–cement interface as an infinite thin layer characterized by its thermal conductivity only, thus leads to underestimation of the predicted maximum bone temperature. For example, Mazzullo et al. (1991) calculated a peak bone temperature to be 57°C, which is clearly much less than the maximum temperature that we find in this study. Similarly, neglecting the bone–cement interpenetration will also lead to an underestimation of peak monomer leftover concentrations. As we demonstrated in this study, this concentration can be as high as 15% near embedded trabeculae. Although the average monomer leftover concentration found in this study (4–5% in the bulk) is in the same range as values usually reported (Kühn, 2002), the actual local concentration thus can be much higher.

We conclude that modelling the bone microstructure is essential for the calculation of accurate temperature and monomer leftover profiles for bone tissues. Presently, we do not know whether the actual microstructural geometry has a large effect on the calculated profiles. It is interesting to note, though, that the generic 2-D micro-model used in the early study of Huiskes (1980) predicted similar temperatures for the bone tissue enclosed in the cement (up to 78°C) as is found in the present study, suggesting that the actual microstructure might have only a minor effect on the results. Unfortunately, this earlier study did not account for the interface heat capacity nor for the cement polymerisation kinetics, making it difficult to compare results presented there with those obtained in our study.

We also found, that the bone tissue that is subjected to the highest temperatures is also subjected to high leftover monomer concentration. Furthermore, the maximum bone temperature is reached relatively early, when monomer content in the neighbouring cement is still quite high. Available experimental data on the effect of the monomethylmethacrylate monomer on the bone tissue demonstrate its toxic effects (e.g. Willert et al., 1974; Linder, 1977). Thermal necrosis has been reported in bone tissue exposed to temperatures in excess of 50°C for more than 1 min (Eriksson et al., 1984; Rouiller and Majno, 1953). It thus seems unlikely that cells subjected to the conditions found here will survive and necrosis is expected. Trabeculae embedded in the cement, however, cannot remodel, and it thus is likely that the bone–cement interface will remain intact and capable of...
load carrying, at least as long as no (micro-) fractures occur.

The model, developed by Mazzullo et al. (1991), that was used in this paper is one of the most advanced PMMA polymerisation models capable of modelling the monomer leftover. This is not possible with the more recent model of Baliga et al. (1992) that has been used in several later studies (Starke et al., 1998, Lennon et al., 2002). Very recently, Hansen (2003) proposed a more advanced model that includes the separate modelling of initiation and chain growth phases of the polymerisation process. Although such models can probably further refine and improve the results, we feel that the model used in this study was adequate for our purposes.

Some limitations of the present model need to be discussed. Although the geometry of the bone–cement interface modelled here was obtained from 3-D measurements, it is not clear if it is representative for the bone–cement interface found around cemented implants or after vertebroplasty. The interface will depend on the bone structure, the preparation of the bone, the consistency of the cement, the pressure applied to it when inserted and on the presence of blood, water and bone debris. In the present experiment the specimen was cleaned of surface marrow and debris left over from cutting, dried and cleaned again. Such a thorough procedure is perhaps not possible in the operating room. Consequently, the cement penetration found in this study is expected to be higher than in clinical practice. Ishihara et al. (2002) report that cement penetration depth is relatively insensitive to cement pressure, but washing of the bone surface prior to cement application increases this depth and increases mechanical strength of the interface. Therefore maximum cement penetration is usually regarded as a goal to achieve in orthopaedic operations. The effects considered in the present paper may play a vital role then.

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