Thermodynamical finite element analysis of self-curing bone cement

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CHAPTER 14

Thermodynamical Finite Element Analysis of Self-Curing Bone Cement (PMMA)

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A mathematical model, based on thermodynamical principles, was developed to analyse non-steady heat generation and conduction in self-curing acrylic cements, as used in orthopaedic surgery. The equations that describe the model are solved with time discretization and finite element methods; the model takes three-dimensional geometrical and thermodynamical properties of all materials (bone, cement, implants) into account.

The model can be used to predict the non-steady temperature distribution in bone during implantation procedures and to evaluate the influences of thermodynamical and geometrical properties on heat generation and conduction in various circumstances.

This chapter outlines and evaluates the analysis method.

Although orthopaedic joint surgery has been reasonably successful during recent years after the introduction of bone cement (polymethylmethacrylate) for implant fixation, side effects may still lead to complications such as necrosis of the bone surrounding the cement; this is sometimes irreverisible and may result in the prosthesis loosening.[1]

Feith[2] used rabbits in experiments to analyse the adverse side effects of the acrylic cement. He concluded that mechanical damage to the blood circulation and the cytotoxic effects of the monomer were minor, and that the principal cause of the tissue reactions was the high curing temperature of the commercial cements. This high temperature results from the heat that is generated within the mixture, while the monomethylmethacrylate (monomer) polymerizes to polymer chains. The heat is conducted through the implanted prosthesis and the bone. *In vivo* temperatures measured at the cement–bone interface varied between 40 and 90°C;[3–8] composition of the mixture, quantities used, geometrical configurations, and initial and ambient temperatures proved to have important influences on the results. Because of the steep temperature gradient in the bone[6] the position of the thermocouples is critical, which could explain the variety in reported values. Temperatures were also measured under various conditions in laboratory experiments;[3,7,9–11] maximum temperatures measured in curing cement masses could be as high as 150°C. These experiments showed again that the temperature values depend greatly on the geometrical and thermodynamical parameters of the materials used.

The object of this study was to analyse the influences of these parameters on the heat generation and conduction in the materials under various conditions. A mathematical model was developed to describe the thermodynamic process, taking into account the important thermodynamical and geometrical properties of the different materials and the curing properties of the cement. Mathematical models used were: a one-dimensional model of heat conduction across interfaces;[11] a one-dimensional finite difference model of heat generation and conduction in an endlessly long cylindrical construction of prosthesis, cement, and bone;[12] and an axisymmetric finite element model to describe heat conduction in a construction of bone, cement, and prosthesis.[13] The first was used to calculate the cooling velocity at the interfaces, the second and the third to evaluate temperatures in cement and bone after implantation of hip endoprostheses and to analyse the influence of the thickness of the cement layer.

METHODS

It is assumed in the model that the materials are non-compressible and that their properties are isotropic and independent of temperature, that there is no convection in the materials, and that the geometry is axisymmetric (although not cylindrical).

The model can then be described by the following differential equation:[14]

$$\frac{1}{r}\cdot\frac{\partial}{\partial r}\left(\lambda\cdot r\cdot\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(\lambda\cdot\frac{\partial T}{\partial z}\right)-a\cdot\frac{\partial T}{\partial t}+\Phi=0$$

where t = time (sec); $a(r,z)$ = mat. parameters (sec/m^2); r, z = coordinates (m); $\phi(r,z,t)$ = heat source (J/m^3 sec); $T(r,z,t)$ = temperature (°C); and $\lambda(r,z)$ = conductivity (J/sec degC m).

The parameter $a(r,z)$ can, for each material, be evaluated from $a=\rho c$, where $\rho(r,z)$ = density (kg/m^3) and $c(r,z)$ = specific heat (J/kg degC).

The part of the monomer in the cement mixture that has polymerized at a certain time is denoted by $p(t)$ and called the 'polymerization curve'. The heat generated in the monomer is proportional to the derivative dp/dt of the polymerization curve, because of the kinematics of the polymerization.[15] The proportionality constant is dependent on the total amount of heat generated in a unit mass of monomer and the amount of monomer in the

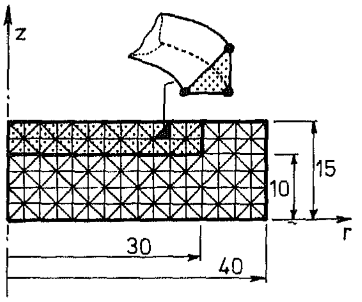

Figure 1. Element mesh of a quarter part of a Teflon cup (see Figure 2) with cement.

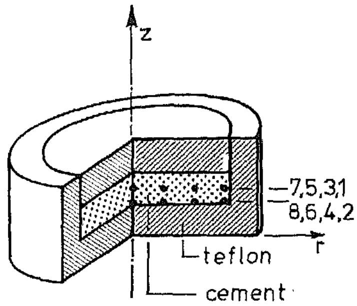

Figure 2. Teflon cup filled with cement as used by Meyer. Measuring points 1 through 8 are marked. (Measuring points 2, 4, 6, and 8 are located 0.5 mm from the interface.)

mixture, so that:

$$\Phi(t) = \frac{\rho_m}{1+\gamma_v} \cdot Q_t \cdot \frac{dp}{dt}(t)$$

where ρ_m = density of MMA (kg/m^3); Q_t = heat production (J/kg MMA); γ_v = volume ratio PMMA/MMA; and $p(t)$ = polymerization curve.

As for the boundary condition, it is assumed that either the temperature at a boundary piece of the construction or the heat release to the environment can be prescribed.

The equations that describe the model are, together with the boundary conditions, solved for a construction of different materials by discretization of the time-dependent functions according to Euler's rule and the application of finite element method procedures at every time step;[16,17] the construction is therefore divided into a mesh of ring elements with triangular cross sections (Figure 1).

For this procedure a computer programme was developed by adapting a programme suited for static heat conduction problems.[18] The programme was tried out, with excellent results, for simplified heat generation and conduction problems for which analytical solutions are known.[14]

To verify the model, an experiment reported by Meyer *et al.*[3] was simulated. Temperatures were measured as functions of time at eight locations in acrylic cement, curing in an axisymmetric polytetrafluoroethylene (Teflon) cup (Figure 2).

Because of the symmetry of this construction, only one-quarter of a cross section has to be considered in the simulation.

Parameter values used in the simulation are given in Table 1.

TABLE 1. Parameter values used in the calculations. Numbers in parentheses refer to literature.

Parameter	Value	Ref.	Parameter	Value	Ref.
General			*Teflon*		
Geometry	See Figure 1	(3)	λ_t (J/sec degC m)	0.234	(21)
T_0 (°C)	25	(3)	ρ_t (kg/m^3)	2.2×10^3	(21)
T_u (°C)	25	(3)	c_t (J/kg degC)	1.04×10^3	(21)
Cement			*Bone*		
γ_v (m^3/m^3)	1.68	(3)	λ_b (J/sec degC m)	0.293	(23)
Q_t (J/kg)	4.9×10^5	(19)	ρ_b (J/kg degC)	2.6×10^3	(24)
ρ_m (kg/m^3)	0.94×10^3	(20)	c_b (J/kg degC)	3.05×10^3	(23)
λ_c (J/sec degC m)	0.167	(3)			
ρ_c (kg/m^3)	1.19×10^3	(21)			
c_c (J/kg degC)	1.46×10^3	(21)			

RESULTS

It was established that for a problem of this kind a time step to polymerization time ratio of 0.02 and a mesh of 192 elements (Figure 1) gave good results. Figure 3 shows results of the simulation, temperature *vs.* time in the middle point of the cup, as calculated for four different polymerization curves.

The polymerization curve No. 4, that has the best fit to the experimental

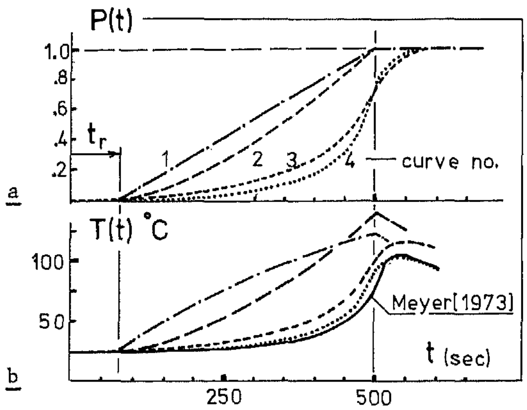

Figure 3. (a) Temperature *vs.* time in the middle of the cup (point 7) as calculated for (b) four different polymerization curves, compared with experimental results.

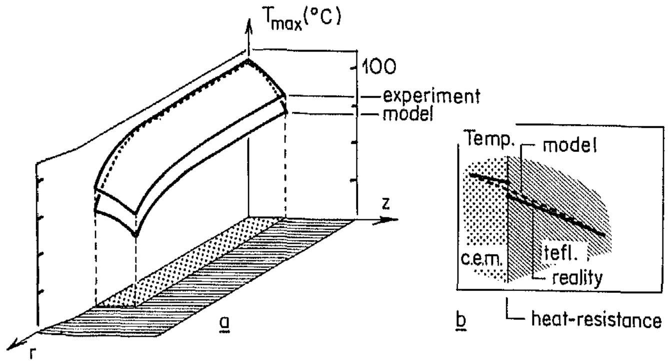

Figure 4. (a) Maximum temperatures in a cross section, as calculated and as measured by Meyer (interpolated). (b) In reality there will be a heat resistance across the interface that is not taken into account by the model.

results, was derived from laboratory measurements of the polymerization process, using a delatometer. A retardation time (t_r) was added and the time values were multiplied with a time-scaling factor (t_s). Both t_r and t_s were evaluated from Meyer's experiment.

Polymerization curve No. 3 was also derived from these delatomer measurements by using only a time-scaling factor, and curves Nos. 1 and 2 are assumptions (the derivative of curve No. 1 is constant in time, that of curve No. 2 is proportional with time).

Figure 4 shows a comparison of calculated and measured maximum temperatures in a cross section of the cup. It could be established that the differences are most likely due to a heat resistance across the cement–Teflon interface that is not taken into account by the model.

Figure 5 compares temperatures calculated at four points on the axis of symmetry, in two different circumstances: (1) where the heat release to the environment is prescribed as zero (ideally isolated); and (2) where the

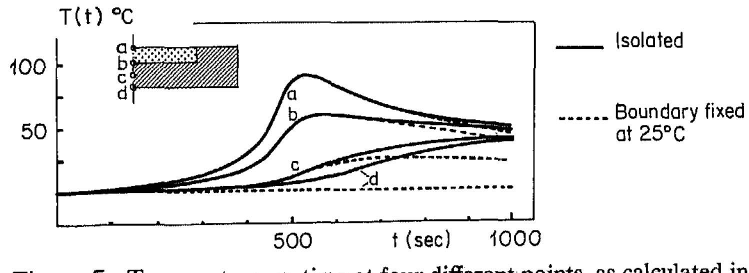

Figure 5. Temperature *vs.* time at four different points, as calculated in two different circumstances (see text).

boundary temperature is prescribed as 25°C (ideal heat transfer). The boundary conditions appear to have little influence on the maximum temperatures, nor do they influence the first part of the temperature curves at points located in the cement and at the cement–Teflon interface.

DISCUSSION

The comparison of calculated and experimental results indicates that the model can be used to analyse the thermodynamics of acrylic cements. It should be remarked that experimental results cannot be expected to be exact. Values for the parameters were taken from the literature, except for the polymerization curve, the general shape of which was measured in our own laboratories. This curve was adapted using retardation time and a time-scaling factor derived from the experiments. The retardation time is dependent on the chemical composition and can easily be evaluated. The time-scaling factor depends on the polymerization time constant, which is most certainly also a function of the temperature.[15] Once the relation between the temperature and the time constant of the polymerization function is known from experiments, it can easily be taken into account by the model. Until then the polymerization curve has to be treated in the analyses as an independent variable. There will also be a temperature influence on the properties of the cement,[22] especially during the first part of the polymerization, when its state changes from viscous to solid. It appears, however, a reasonable approximation to assume these properties to be constant.

Heat resistances at interfaces between different materials should be taken into account by the model, since they will certainly affect those temperature values that are of interest. Once numerical descriptions of these resistances can be evaluated from experiments, refinement of the model in this sense is possible. The model can only describe axisymmetrical (though not only cylindrical) constructions. Refinement to non-axisymmetry is possible, at the cost of considerably more computer space and time. It is felt, however, that the most interesting phenomena in connection with the clinical use of the cement can satisfactorily be studied while axisymmetry is assumed.

The model and the computer programme can be used not only to predict temperature values as functions of time at interesting locations during clinical use of the cement, but also for sensitivity analyses. For example, they may be used to study influences of geometrical and thermodynamical properties on heat generation and conduction.[25,26] Examples of such parameter studies are given with respect to the polymerization curve (Figure 4) and to the boundary conditions (Figure 5).

When the model is used to simulate *in vivo* circumstances the influence of the blood circulation should be taken into consideration, for instance by assuming a prescribed boundary (outside bone) temperature of 37°C. Figure 5 indicates that this will probably not influence the maximum temperatures in the bone near the cement–bone interface, but it will, of course, shorten the time needed for the heat to transfer.

It can be seen in Table 1 that, while the density and the conductivity of bone have the same order of magnitude as Teflon, the specific heat is about three times greater. This means that more heat can be stored in bone with lower temperatures, but also that bone will 'pull' more at the heat generated within the cement. The consequence of this can be studied with the model.

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