A Numerical Model for Temperature Distribution and Thermal Damage Calculations in Teeth Exposed to a CO_2 Laser

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ABSTRACT

A numerical axisymmetrical model which may be used for the evaluation of laser dental treatments is presented. This model facilitates the calculations of the temperature distribution and of thermal damage to pulp tissue caused by CO_2 laser irradiation. Temperature distributions are compared with analytical, experimental, and numerical results presented in the literature. The conformity obtained is good. It is shown that this model can be used over a wider range of time intervals and physical conditions than a previous numerical model. In addition, thermal damage is calculated for the temperature distributions presented in this paper. This model can be utilized for the optimization of exposure parameters to minimize pulp damage in the application of lasers for dental treatment.

NOTATION

T = temperature (°C)
T_∞ = environmental temperature (°C).
t = time (sec)
k = thermal conductivity (W/cm °C)
c = heat capacity (J/g °C)
ρ = density (g/cm^3)
α = thermal diffusivity (cm^2/sec)
L = tooth length (cm)
z = depth (cm)
R_T = tooth radius (cm)

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F_0 = uniform heat flux at the semiinfinite body surface (W/cm^2)
I_0 = power density at the center of the laser beam (W/cm^2)
w = laser beam radius (at which the intensity is $1/e^2$ of the peak intensity) (cm)
r = radial distance from symmetric axis (cm)
β = absorption coefficient (cm^{-1})
ΔE = activation energy (J/mole)
A = process constant (sec^{-1})
ε = emissivity
σ = Stefan-Boltzmann constant = 5.65×10^{-12} $W/cm^2\,°C^4$
h = convection coefficient ($W/cm^2\,°C$)
R = universal gas constant = 8.314 J/mole

SUBSCRIPTS

d = dentin
e = enamel
p = pulp

INTRODUCTION

Since its introduction in 1960, the laser has fascinated many physicians, who have searched for applications in medicine. In 1964 Stern and Sognnaes [21] reported that the ruby laser pulse could evaporate enamel, leaving behind a fused glasslike crater. With the development of other lasers a period of intense research ensued, as summarized by Stern [22] in 1974. The conclusion of this summary was that the laser will probably never replace totally the dental drill, but its effects might prove helpful in tempering the outer layers of enamel of the tooth to withstand demineralization and caries [19,23]. A number of publications [2,16,24,25,27,28] suggest the possible development of preventative dental methods, which include:

(a) Sterilization of caries or demineralized enamel zones [16].
(b) Fluoride uptake enhancement by the enamel matrix [2].
(c) Use of new durable pit and fissure sealants on the tooth surface [2].

In spite of these promising applications and the common use of lasers in surgery and therapy today, their potential has not been properly realized clinically by dentists. The main reason for this lag is the fear of causing thermal damage to the pulp [22]. Very high temperatures are generated at the exposed site, and the heat conduction from these areas can cause irreversible damage to the temperature sensitive pulp.

A wide range of energies and power densities are produced by the different methods of dental treatment, and an accurate assessment of the temperature rise and the thermal damage to the pulp is required in each case. Experimental work on analysis of the thermal damage has shown results ranging from destructive thermal damage [26] to partial damage [1] to virtually no significant damage [16].

In this work, a numerical model is developed to facilitate the calculation of the temperature distribution on the tooth surface and within its volume and the evaluation of the thermal damage caused by different laser treatments. The model developed is axisymmetrical, employing the method of finite differences to approximate the spatial part of the heat equation. Integration is performed by variable step integration methods to the accuracy required. The model describes the thermal behavior of molar teeth, irradiated on the crown, assuming cylindrical geometry. Many cases of exposed tooth surfaces can be evaluated by approximation to a semiinfinite body: namely, exposures to short pulses of beams which are narrow compared to the curvature and size of the tooth surface.

As far as is known today, no reliable tool exists that could provide a quantitative assessment of the degree of damage sustained by the pulp for laser dental treatments. The model presented uses the temperature field to estimate the thermal damage, assuming it to behave as a temperature sensitive rate process.

THE NUMERICAL MODEL

The purposes of the model are to:

(a) Evaluate the temporal and spatial variations of the temperature in the tooth as a result of a laser action on its surface.

(b) Provide a quantitative assessment of the thermal damage to the pulp at any point.

(c) Analyze the effect of different exposures of the tooth to the laser beam (single pulse, train of pulses, continuous wave).

In addition, the model should be simple to use and flexible enough to permit variations of parameters for specific needs.

The knowledge of the thermal properties of the dental tissues and understanding the laser-tissue interaction is required in order to obtain accurate results.

The CO_2 laser's absorption coefficient in biological tissue is not known accurately and is assumed to be very high [2,22]. In these works the laser absorption is considered to occur on the surface only. Duley [10] obtains for organic solids an absorption coefficient range of 10^2–10^4 cm^{-1}. It follows that a value of 10^3 cm^{-1} can be chosen as a first approximation. Due to this small absorption depth, the internal scattering coefficients can be neglected [11]. The CO_2 laser beam is absorbed by molecular excitation of vibrational levels of the medium, the lifetime of which is smaller than 10^{-12} sec [18]. This means that the energy conversion period is extremely short compared to

TABLE 1

Thermal Coefficients Chosen for the Tooth Tissues

	k W/cm °C	c J/g °C	ρ g/cm^3
Enamel	9.34×10^{-3}	0.71	2.8
Dentin	5.69×10^{-3}	1.59	1.96
Pulp	4.19×10^{-3}	3.77	1.05

conventional laser pulse durations. It may thus be assumed that the absorbed laser energy is the heat source in the analyzed medium. No information is available on the reflection of the CO_2 laser beam from the tooth surface. Stern [22] and Boehm [3] assumed a very small degree of reflection of the CO_2 10.6 μm radiation from the enamel surface. In their works they used a zero reflection coefficient approximation. In the present work, this assumption was adopted for the sake of comparison.

Whenever used in this work, the emissivity of the dental enamel is taken to be equal to 1. This is a reasonable assumption because of the very high absorption of infrared wavelengths by enamel [3,22]. Also, emissivities for similar materials are known to be close to this value [15].

In a similar manner [5], a representative value for the convection coefficient is chosen to be $h = 0.031$ W/cm^2 °C. The thermal characteristics of hard dental structures were tested by Brown et al. [7]. As for the soft pulp tissue, it may be assumed to behave thermally like connective tissue [22], or with a good approximation to have the average of thermal coefficients of soft tissues [6,9]. From data in the literature [6,7,9] we have chosen the coefficients as presented in Table 1, where k, c, and ρ are the thermal conductivity, heat capacity, and density, respectively.

As can be seen from Table 1, the tooth tissues are poor heat conductors. Thus, it should be advantageous to choose a model that enables a semiinfinite body approximation for narrow laser beams and short pulse durations.

An axisymmetrical model was chosen in which the geometry is cylindrical. The laser beam irradiates the top cylindrical base along the same symmetrical axis, Fig. 1. This model simplifies a 3-D problem into a 2-D problem and also provides a close approximation of the molar tooth geometry.

The governing equation is

$$\rho(r,z)c(r,z)\frac{\partial T(r,z,t)}{\partial t} = \nabla[k(r,z)\nabla T(r,z,t)] + S(r,z,t), \quad (1)$$

where T is the temperature and S includes all the heat sources. It is assumed that the thermal properties in this case are temperature independent. How-

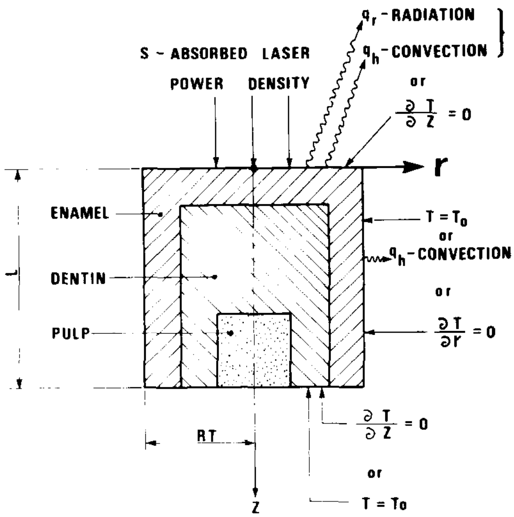

FIG. 1. General axisymmetrical model with all possible boundary conditions.

ever, since the model might be composed of three different tissue components, with geometries as defined in Figure 1, there is a spatial dependence of the thermal properties.

The initial condition is

$$T = T_0 \qquad \text{at} \quad t = 0. \tag{2}$$

The boundary conditions are defined schematically in Figure 1. Although energy losses caused by thermal radiation and convection can be neglected in most cases, it is possible to choose any set of boundary conditions to enable more accurate solutions for special cases.

The heat source is assumed to be the absorbed energy of the laser (operating at the TEM_{00} mode) and is defined as

$$S = I_0 \exp\left(-\frac{2r^2}{w^2} \right) \qquad \text{(laser on)}, \tag{3.a}$$

$$S = 0 \qquad \text{(laser off)}, \tag{3.b}$$

where I_0 is the power density at the center of the laser beam, w is the beam radius (at which the intensity is I_0/e^2), and r is the radial distance from the symmetric axis. The thermal radiation is

$$q_r = \varepsilon\sigma \cdot \left(T^4 - T_\infty^4 \right), \tag{4}$$

where ε is the emissivity, $\sigma = 5.65 \times 10^{-12}$ W/cm^2 °C^4 is the Stefan-Boltzmann constant, and T_∞ is the environmental temperature. The convected energy is

$$q_h = h(T - T_\infty). \tag{5}$$

With the subscripts e, d and p, for the enamel, dentin and pulp, respectively, the continuity conditions are defined at the dentin-enamel boundary by

$$T_d = T_e, \tag{6.a}$$

$$k_d \frac{\partial T_d}{\partial r} = k_e \frac{\partial T_e}{\partial r}, \tag{6.b}$$

$$k_d \frac{\partial T_d}{\partial z} = k_e \frac{\partial T_e}{\partial z}, \tag{6.c}$$

and at the pulp-dentin boundary by

$$T_p = T_d, \tag{7.a}$$

$$k_p \frac{\partial T_p}{\partial r} = k_d \frac{\partial T_d}{\partial r}, \tag{7.b}$$

$$k_p \frac{\partial T_p}{\partial z} = k_d \frac{\partial T_d}{\partial z}. \tag{7.c}$$

The spatial part of Equation (1) is approximated by finite differences. The CSMP software package [20], which is utilized to handle this model, facilitates simple and efficient changes of the exposure conditions. Depending on the accuracy needed, the temporal integration step can be changed automatically by a variable step Runge-Kutta (fourth order) method, or by a variable step Milne (fifth order) method.

The grid size $(\Delta r, \Delta z)$ used in this model can be varied in different fashions. For the calculations made in this work, a variable grid size is utilized. The grid is very small close to the surface and the axis of symmetry $(z \to 0,\ r \to 0)$ and increases gradually along r and z. This variable grid was adapted because of the enormous temperature gradients developed at the laser exposed site and the decrease of these gradients as z and r increase.

The temperature distribution results are used by the model to calculate the thermal damage caused to the soft dental tissue. Soft tissue exposed to heat will undergo thermochemical changes by denaturization of enzymes and proteins. This temperature and time related phenomenon can be described by a rate process equation derived from the Arrhenious equation [14]:

$$\frac{d\Omega}{dt} = A \exp\left[-\frac{\Delta E}{R(T + 273°)} \right] \tag{8}$$

where Ω is a function defining quantitively the thermal damage, ΔE is the activation energy, A is a process constant, and $R = 8.314$ J/mole is the universal gas constant. By integration,

$$\Omega = A\int_0^t \exp\left[-\frac{\Delta E}{R(T+273°)}\right] dt \tag{9}$$

Henriques and Moritz's publications on this subject [12,13,17] present an important contribution in this field. Henriques [13] assumed for pigskin and subcutanous tissues that the damage mechanism can be described as a single rate process (although several processes with different rates might be involved). From experimental results the authors determined values for ΔE and A. These values describe a single rate process in the range extending from intact tissue to destruction amounting to complete tissue necrosis. The values obtained were $\Delta E = 628{,}020$ J/mole and $A = 3.1 \times 10^{98}$ sec^{-1}, where in the range:

(a) $\Omega \geqslant 1$, complete epidermal necrosis occurs;
(b) $1 > \Omega \geqslant 0.53$, irreversible damage effects begin to occur;
(c) $\Omega < 0.53$, no irreversible damage will occur.

In order to assess the thermal damage to the pulp, Equation (9) is utilized for each point in the tooth. For a first approximation, the values of ΔE and A as given above are used. Further histological experimental work is required for better determination of those values for the pulp.

RESULTS

1. *COMPARISON OF THE MODEL RESULTS WITH ANALYTICAL RESULTS*

When treating the tooth, the extent of thermal damage to the pulp resulting from the thermal processes on the tooth surface should be known. These surface thermal processes will depend on the required clinical results, e.g., the minimal temperature for enamel tempering or for the sterilization of caries. Thus, it is important to evaluate the model's capability to predict surface temperatures. For this purpose the model results are compared with analytical results. Consider a 1-D insulated semiinfinite body, with a heat source given by

$$S(z) = F_0 e^{-\beta z}, \tag{10}$$

where F_0 is a uniform heat flux (at the semiinfinite body surface) and β is the absorption coefficient, and with an initial condition of

$$T = 0 \quad \text{at} \quad t = 0. \tag{11}$$

The analytical solution of the heat equation is given by [8,18]

$$T(z,t) = \frac{2F_0}{k}(\alpha t)^{1/2} i\,\mathrm{erfc}\left[\frac{z}{2(\alpha t)^{1/2}}\right] - \frac{F_0}{\beta k} e^{-\beta z}$$
$$+ \frac{F_0}{2\beta k}\exp(\beta^2 \alpha t - \beta z)\,\mathrm{erfc}\left[\beta(\alpha t)^{1/2} - \frac{z}{2(\alpha t)^{1/2}}\right]$$
$$+ \frac{F_0}{2\beta k}\exp(\beta^2 \alpha t + \beta z)\,\mathrm{erfc}\left[\beta(\alpha t)^{1/2} + \frac{z}{2(\alpha t)^{1/2}}\right] \qquad (12)$$

where α is the thermal diffusivity, defined as $\alpha = k/\rho c$. This solution can be used as a good approximation to the laser heating if:

(a) The heat source is considered to be the laser absorbed energy, with an absorption coefficient $-\beta$.

(b) The laser beam is very wide compared to the depth of interest and has a uniform power density throughout its cross-section.

By examining Equation (12), it may be seen that besides the temperature dependence on the energy flux and the thermal characteristics, there is a dependence on the absorption coefficient $-\beta$. In order to simplify the calculations for the numerical model, it is assumed that the laser absorption is uniform in the volume of pixel elements which are bounded by the outer surface ($z = 0$). As depicted in Equation (3.a), each pixel receives a portion of energy depending on its distance from the laser beam axis. Small pixel elements are required near the absorption surface ($z = 0$) if accurate surface temperatures at short time intervals are needed. For time intervals of the order of 10^{-2} sec and for an absorption coefficient of 1200 cm^{-1}, an absorption slab thickness of $3.5/\beta$ is chosen (this slab will absorb 97% of the energy radiating through the $z = 0$ surface). The 1-D semiinfinite body approximation can be simulated by the numerical model. This is done by increasing the laser beam diameter to a value much larger than the tooth size and examining the temperatures at point in the region around $z \to 0$, $r \to 0$.

Figure 2 shows the surface temperature profiles as given by the analytical and numerical solutions. The conformity of the results is found to be good.

Numerical and analytical results are also given for small depths, where the semiinfinite model can still be approximated. These results for depths of 0.003, 0.006, and 0.0074 cm are also shown in Figure 2, to prove a good fit between the results. All results in Figure 2 were calculated using the parameters given in Table 2. Since the analytical solutions can be used only for a very small range of physical conditions (e.g., very small depths and very wide laser beams), the numerical model results should be compared with solutions in a wider range of physical conditions.

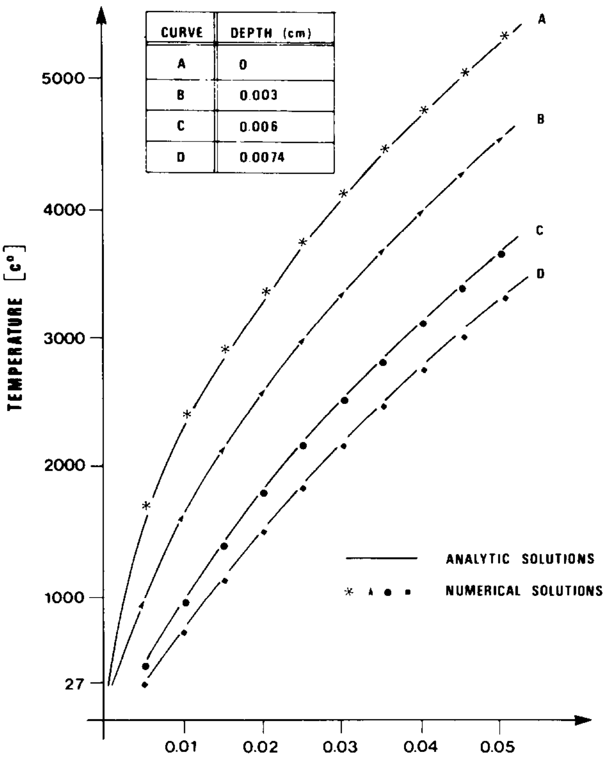

FIG. 2. Comparison of the model numerical results with analytical results for surface temperature and for temperature at small depths during laser exposures.

TABLE 2

Physical Properties and Exposure Parameters Used to Calculate the Results in Figure 2.

$k = 6.28 \times 10^{-3}$ W/cm °C
$c = 1.17$ J/g °C
$\rho = 1.5$ g/cm^3
$I_0 = 2219$ W/cm^2
$F_0 = 2219$ W/cm^2
$\beta = 1200$ cm^{-1}
$w = 20$ cm
Tooth radius = $R_T = 0.3$ cm
Tooth length = $L = 0.6$ cm

2. *ANALYSIS AND COMPARISON WITH PUBLISHED NUMERICAL RESULTS*

Boehm et al. [4] developed a numerical model to evaluate the temperature distribution in the tooth, following pulsed CO_2 laser irradiation. It is reported that difficulties were encountered in numerically calculating the temperature on the exposed surface during and immediately following irradiation. For short time ranges ($t <$ pulse duration) no information is provided. The thermal properties for the hard dental tissues used by Boehm are the same as given in Table 1. Thus, these data are used also in the present model in the calculations.

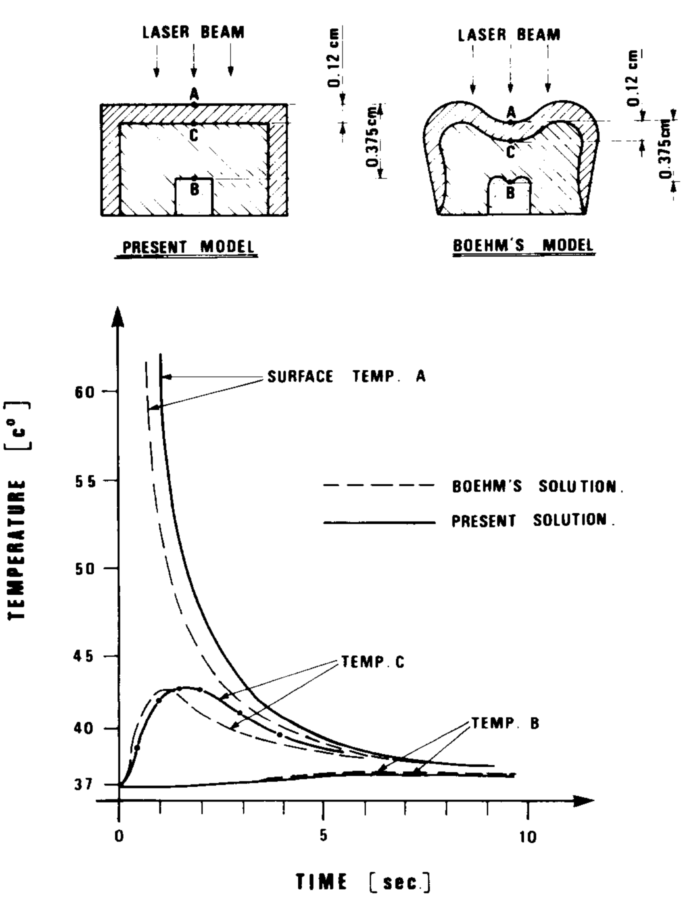

FIG. 3. Comparison of the model results with Boehm's numerical results [4] for: (a) the exposed surface, (b) the pulp-dentin junction, and (c) the enamel-dentin junction. Exposure parameters: absorbed energy 0.7 J, beam diameter 0.26 cm, pulse duration 2.4×10^{-6} sec.

Figure 3 shows the temperature profiles at the irradiated surface (a), at the enamel-dentin boundary (c), and at the pulp-dentin boundary (b). There is a good fit between the results inside the tooth. On the surface, the temperature given by the present model is slightly higher than Boehm's results, but the differences increase at shorter time intervals. It is particularly important to evaluate the exact surface temperature, in order to understand the thermal processes occurring on the tooth surface. Thus, the solution is extended to the short time intervals, as shown in Figure 4. Using the same physical assumptions [4] that there are no heat losses due to water evaporation, thermal radiation, or convection, and assuming that the enamel is not limited in reaching high temperatures, an increase of 4600°C is found at the end of the pulse. This high temperature is more than four times larger than the temperature presented by Boehm for times shorter than 10^{-4} sec. However, it is still about 29% lower than that calculated from the analytical formula, Equation (12), which incorporates the characteristic absorption coefficient $\beta = 1000$ cm^{-1}. This deviation from the analytical solution is expected and stems from:

(a) The absorption mechanism used is a uniform volume absorption and not one following Beer's law. This influences results at very short times before diffusional effects become important.

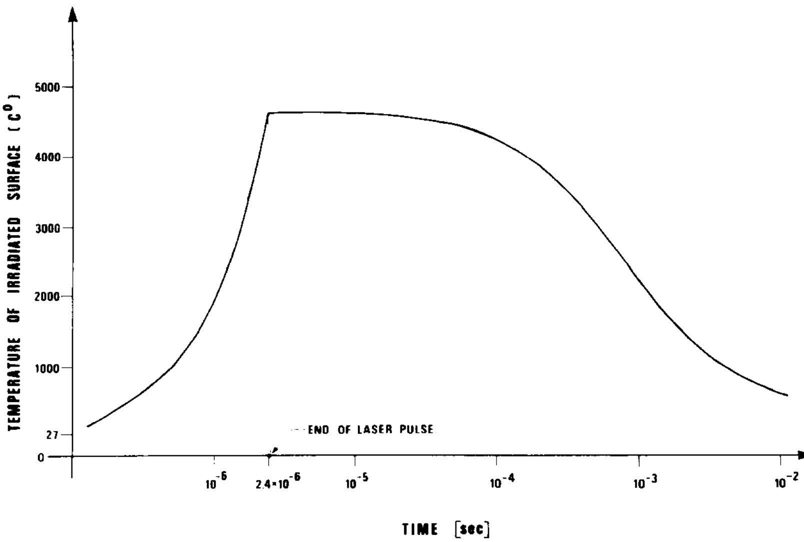

FIG. 4. Temperature profile of the exposed surface, in a short time interval during and after pulsed laser irradiation (model results for the Boehm's case [4] simulation).

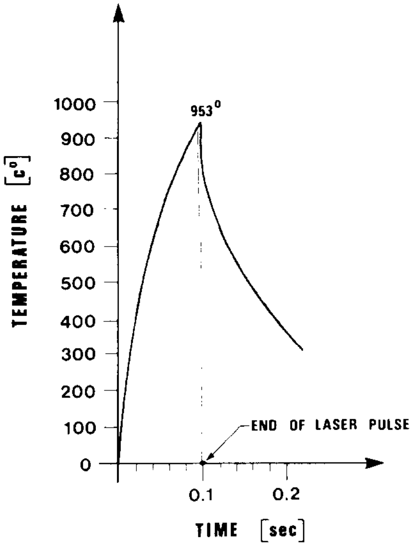

FIG. 5. Temperature profile of the exposed surface for the Suzuki-Tomita experiment [25,27] simulation. Exposure parameters: absorbed energy 10 J, beam diameter 0.8 cm, pulse duration 0.1 sec.

(b) The numerical model simulates a gaussian laser beam. The beam's peak power density is equal to the uniform heat flux on the analytical model surface. Also, the beam's radius is smaller than the tooth radius. This results in a radial temperature gradient on the surface; hence a radial heat flow exists and a larger temperature rise of the examined point is prevented.

3. *COMPARISON WITH EXPERIMENTAL WORK*

Suzuki and Tomita [25,27] presented in 1981 their experiments on the changes that enamel undergoes when irradiated with low power density CO_2 laser beams. They exposed the enamel with laser pulses of 5–10 J, 8 mm beam diameters, for durations of 0.1–0.2 sec. As a result, they obtained a decrease of the enamel permeability to demineralization, with an enamel surface that remained smooth, without flakes and with sealing of micropores by a melting process. Studying the crystallographic and chemical binding state changes and the resistance to acid, they found that these changes are the same as those created by heating tooth enamel to 1000°C.

Simulating their experiment with 0.1 sec pulses of 10 J energy and 8 mm diameter yields the surface temperature profile given in Figure 5. The maximal temperature rise is 953°. Assuming an initial temperature of

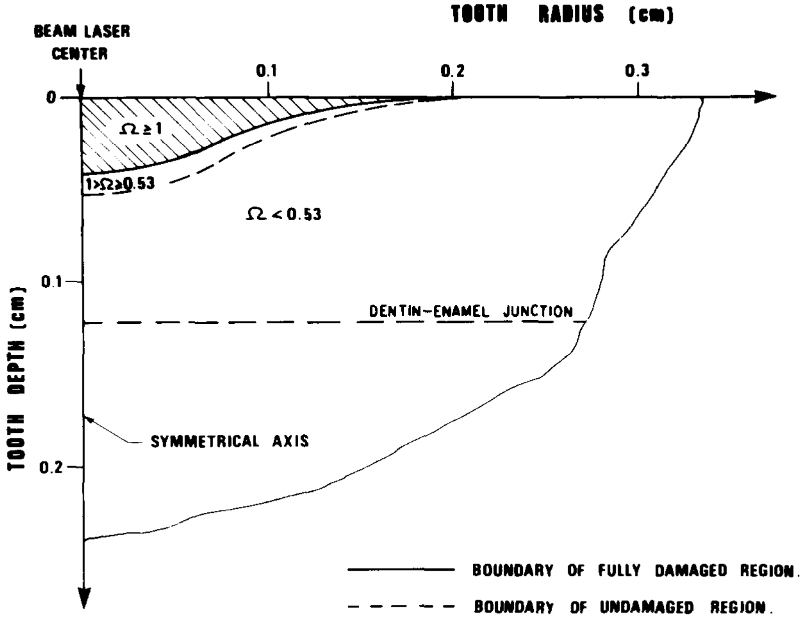

FIG. 6. Thermal damage distribution for simulation of Boehm's data [4]. Exposure parameters: absorbed energy 0.7 J, beam radius 0.13 cm, pulse duration 2.4×10^{-6} sec.

20–37°C, the maximal surface temperature will reach 973–990°C. This numerically calculated temperature is very close to the 1000°C, which causes similar thermal changes on enamel surface to those reported by Suzuki and Tomita. This result further confirms the power and accuracy of the proposed model.

4. *ANALYSIS OF THE THERMAL DAMAGE MODEL*

Thermal damage maps are shown in Figures 6, 7, 8. The thermal damage distribution is represented by plotting on the tooth cross-section the boundaries of zones for which the damage function Ω is calculated.

It is clear that the exact location and shape of the damage boundaries in these figures depend on the grid resolution used in the model. It is expected, however, that by increasing the grid resolution one will get a smaller transition zone volume, while the $\Omega \geqslant 1$ and the $\Omega < 0.53$ volumes will increase accordingly. In Figure 6, the damage distribution for Boehm's case is presented. This figure shows that the undamaged zone extends up to 0.05 cm from the irradiated tooth surface, while the pulp upper edge is 0.375 cm away from this surface (Figure 3).

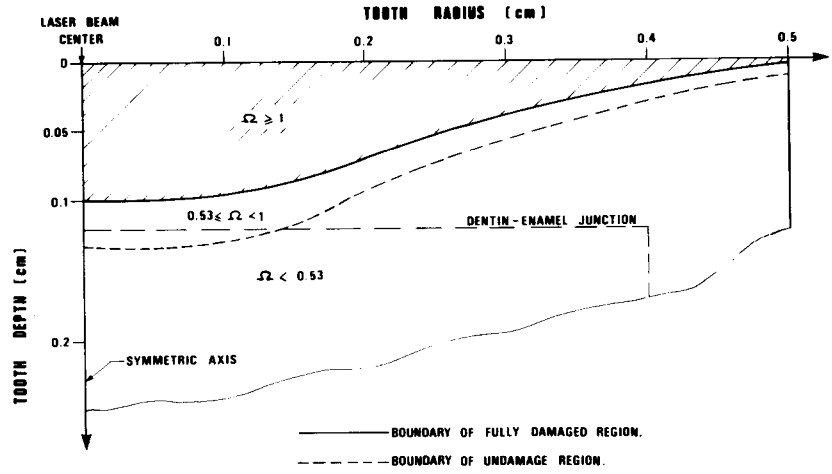

FIG. 7. Thermal damage distribution for the Suzuki-Tomita experiment [25,27] simulation. Exposure parameters: Absorbed energy 10 J, beam radius 0.4 cm, pulse duration 0.1 sec.

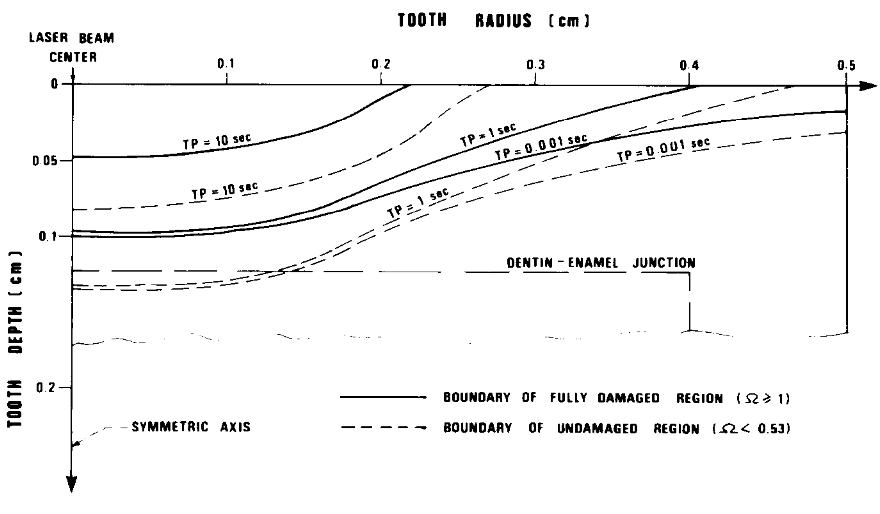

FIG. 8. Thermal damage distribution for different pulse durations. Exposure parameters: absorbed energy 10 J, beam radius 0.4 cm, pulse durations (T_P) 10, 1, and 0.001 sec.

In Figure 7, the thermal damage distribution for soft dental tissue is presented, using Suzuki and Tomita's input parameters as described above. It is found that the total damage zone occupies at its maximum a depth of 0.1 cm.

In Figure 8, three damage distributions are shown for a delivered energy of 10 J for 0.001, 1, and 10 sec pulse durations. It is shown that on increasing the power density, the depth of the damaged zone increases up to a certain limit. This is expected, because as the laser pulse duration is increased and the power densities are decreased, the thermal conductivity mechanism competes more efficiently with the laser power source in the temperature buildup, and the temperature rise is decreased.

CONCLUSIONS

A numerical model, which can be used for evaluation of laser dental treatments, is presented. This model facilitates:

(a) Analysis of different laser exposures on a tooth surface and their thermal effects.

(b) Evaluation of the thermal damage to the dental pulp, using different treatments.

(c) Optimization of laser exposure parameters, for the most effective treatment with the least thermal damage.

The model solutions were compared with analytical solutions for surface and small depth temperature profiles. The temperature rise of the irradiated surface was also compared with reported experimental work [25,27]. A comparison of results for surface temperature and for temperatures deep in the tooth was made with other published numerical results [4]. These comparisons support the model accuracy in calculating the temperature distribution at every point in the tooth. For the thermal damage calculations, the model uses the temperature distribution results, while the damage parameters are taken from data published in literature. Histological work is needed to determine more accurately the damage parameters for pulp, in order to define the damage regions more accurately. This may allow the safe use of wider range of laser treatments even with smaller safety margins.

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