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Application of CFD Simulation to Localized Cure pHEMA Using Infrared Laser

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The poly 2 - hydroxy ethyl methacrylate (pHEMA) is a hydrogel very versatile in the field of medicine, due to its properties of biocompatibility, similar to the soft tissues of the body. It is easy to prepare and can be applied as substitute natural articular cartilage. For this application the use of infrared laser allow to irradiate the polymer and obtain the localized cure with the required design and properties of the final product. In order that, it becomes important to have a well established and controlled process so that it is possible to have rapid and localized cure of polymer to prevent the dissipation of energy in unwanted regions. This is a necessary issue where the goal is the replacement of articular cartilage in regions with specific geometries. Bearing all these in mind, in this work is proposed and used a simulation tool to predict, and diagnose the temperature distribution during the localized cure of pHEMA. This allows determining the operating parameters of the process, such as temperature and curing time and laser power. These parameters were entered into the system with infrared laser and were able to get the pHEMA hydrogels by radiation of solutions of 2-hydroxy ethyl methacrylate (HEMA) with data previously determined by simulation. The computational tools make use of fluid dynamics (CFD) implemented in ANSYS CFX ®.

1. Introduction

The advances in modern medicine combined with engineering techniques are creating conditions to restore or even improve the original conditions of the human body by the development of new technologies for application in biomedical devices. One of the techniques currently studied is the use of industrial rapid prototyping technology (3D printing) to materialize structures layer by layer of biomaterials (Jardini et al, 2010). In this technique, the coating of specific geometries requires control of process variables in located curing of the biomaterial (pHEMA, in this case). Thus, the study of temperature distribution in the sample is necessary to prevent radiation of heat in unwanted areas when the sample is subjected to laser beam. This requires the search for optimized operating conditions of the process so that the product of the desired properties may be achieved. To this it was used the numerical method CFD (Computational Fluid Dynamics) to predict the performance of material and to study the impact of process

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operating conditions before its application in the process of the product fabrication. The application of CFD in analysis of fluid flows, in biomaterials, is diverse: analysis of blood pumps (Fraser et al, 2011); microfluidic cell culture system (Huang et al, 2010); perfused bioreactor for cartilage tissue engineering (Cinbiz et al, 2010) etc. The aim of this work was then to simulate and evaluate the heat transfer during localized cure of pHEMA with infrared laser source by using ANSYS CFX® software. This study allows to understand the impact of operating conditions in temperature distribution in the solutions of HEMA so that process procedures and operating conditions may be defined in a optimal or almost optimal fashion in order to obtain the final product with the desired specification.

2. Methodology

2.1 Computational Simulation to Localized Cure pHEMA

The computer simulation helps to solve complex problems through a suitable mathematical model describing the main phenomena taking place taking into account the general boundary conditions. Thus it is possible to reduce cost and time of the analysis by the determination of operating parameters of the process. In this paper, a three-dimensional mathematical model was proposed and solved by the Finite Volume Method (FVM). The thermal analysis performed follow the model presented by Rezende (2006), which used the heat balance equation obtained from the principle of energy conservation, Equation 1. However, in this work was also considered the natural convection in air phase to verify if this parameter influences significantly in the energy losses.

$$\partial\frac{(\rho h)}{\partial t} + \nabla.(\rho U_s h) = \nabla.(\lambda \nabla T) + S_E \tag{1}$$

Where, h, ρ and λ are the enthalpy, density, and thermal conductivity. U_s is the solid motion advection term and is added only when a solid motion velocity is set. S_E is volumetric heat source (ANSYS, 2006).

2.2 Physical model and mesh

In the physical model presented in Figure 1a was considered the heat source referring to heat generated only in the region irradiated by the laser beam. The effect produced by the laser is influenced by a set of variables such as laser beam diameter, intensity, time of interaction of laser radiation with HEMA and the physical properties.

Equations 2 and 3were applied to determine the amount of volumetric heat generated, q, by laser beam and to attach it to the heat generation term (S_E) in Equation 1, as a function of power (P) and volume (V) of material irradiated by laser.

$$q = \frac{P}{V} \tag{2}$$

(3)

The cylindrical volume (V) considered in the model, where the laser energy is deposited, is a function of the laser beam diameter (2ω) and the depth of optical

absorption of the material (δ), which corresponds to the height of the cylinder, Figure 1a. The depth of optical absorption is a property dependent on the composition of the sample. This magnitude is the distance on the surface, even where it is supposed that the radiation from the laser is absorbed by the material (Jardini, 2004; Barbosa, 2010).
The mesh of corresponding physical model was created and resulted in a mesh of 303.801 elements as Figure 1b.

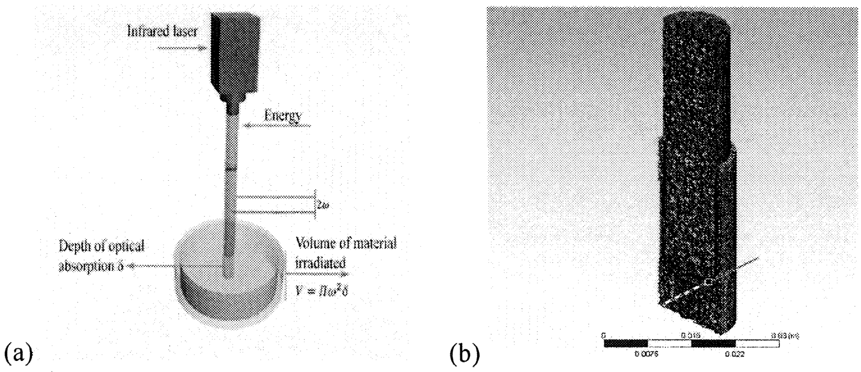


Figure 1. (a) Representation of the physical model; (b) Mesh.

2.3 Boundary Conditions

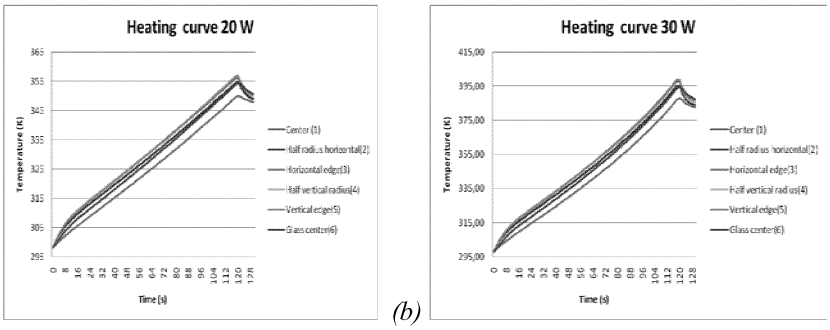
The boundary conditions of CFD model, the operating parameters and the physical properties of the sample and air are presented in Table 1. The heat transfer by radiation was not considered, since this term has a significant influence only for longer periods of thermal analysis and systems at high temperatures. Given this, it was considered initially that the heat transfer occurs by conduction in the HEMA solution and by natural convection from the HEMA solution to the air.
The values of specific heat and thermal conductivity of the solution of HEMA were obtained by the technique of differential scanning calorimetry (DSC) using equipment METTLER TOLEDO DSC 823e. The depth of optical absorption of the solution was determined indirectly by measuring the transmittance using a spectrophotometer model Cary 5G UV-VIS-NIR VARIAN, in the spectral region of near infrared (NIR), from 2500 to 200 nm. The solution density was determined using the Archimedes method, by pycnometer.

Table 1: Boundary conditions, operating parameters and physical properties of the sample

Parameter	Value
Initial temperature of HEMA solution	298 K
Initial temperature of air	298 K
Type of analysis	Transient
Total time	130 s
Time step	1 s
Time of interaction of laser radiation	120 s
Convergence criteria	$1x10^{-4}$
Flow regime	Laminar
Initial composition of the HEMA solution	Dibenzoyl peroxide as thermal initiator: 1% (w/w) and diethylene glycol dimethacrylate as cure agent: 1% (w/w)
Laser power (W)	20 and 30
Laser beam diameter (mm)	8
Thermal conductivity of the solution (W/cm.K)	2,17
Specific density solution (g/cm^3)	1,07
Specific heat of solution (J/Kg.K)	$c_p = 0,0245T + 10,5$
Depth of optical absorption of the HEMA solution (cm)	8,902370267
Thermal conductivity of air (W/cm.K)	0,00026
Specific density of air (g/cm^3)	0,00116
Specific heat of air (J/Kg.K)	1007
Temperature range (K)	295 a 423

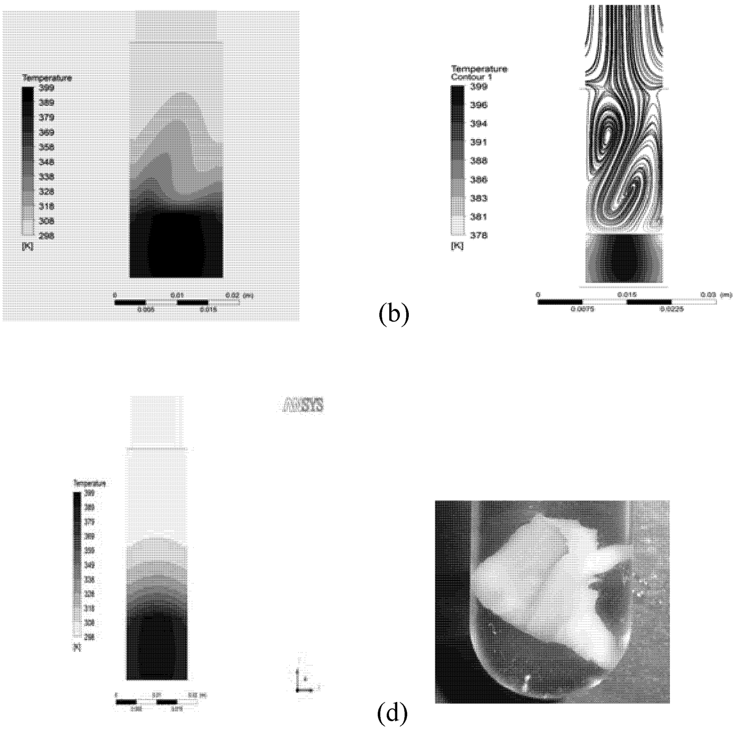
3. Results and Discussion

In the Figures 2a and 2b depict the temperature evolution in six different points (heating curve) during laser irradiation to power of 20 W and 30 W, respectively. The six points discussed in the sample under laser irradiation showed nearly the same temperature profile evolution. It was found that the more removed from the region of incidence of the laser beam (diameter), the lower the temperature reached by the sample (Figures 2a and 2b). Moreover, the greater the power of the laser beam, the higher the temperature achieved in the irradiation of solutions of HEMA. For a laser power of 20 W the maximum temperature reached was approximately 356 K (Figure 2a), while for 30 W the maximum temperature reached was 399 K (Figure 2b), keeping constant the residence time laser in the sample. At a power of 30 W and 120 s was possible to promote the cure of pHEMA. Figures 3a, 3b and 3c show, respectively, the spatial profile of the temperature distribution under effect of conduction and natural convection, the effect of conduction and natural convection and the spatial profile of the temperature distribution in the absence of natural convection, in the HEMA solutions to 30 W power. In the process conditions studied was observed that the natural convection has not significant effect on irradiation of solutions. The Figures 3a and 3c show that it is possible to obtain the same final temperature of the process, 399K, with the effect of convection. Moreover, the presence of convective term in the simulation increased the computational time due to a greater refinement of the mesh and equations included to be solved. Thus, physical model can be simplified suppressing the convective term under these operational conditions and physical properties of the sample. Figure 3d shows the hydrogel de pHEMA obtained via irradiation of a solution of HEMA with the parameters determined by simulation.



(a) *(b)*

Figure 2. Heating curve (a)20 W power (b) 30W power



(a) (b) (c) (d)

Figure 3. (a) Spatial profile of the temperature distribution under effect of conduction and natural convection; (b) Effect of conduction and natural convection (c) Spatial profile of the temperature distribution in the absence of natural convection; (d) pHEMA hydrogel obtained via irradiation laser

4. Conclusions

The use for laser irradiation is one powerful tool to obtain the localized cure in polymers and allows drawing the cured region in specific geometries. The computer simulation allowed determining the parameters of the located cure of pHEMA. It was possible to evaluated the effect of laser power and natural convection in the irradiation samples. It was observed that the temperature of the solution tends to decrease as it moves away from the region of incidence of the laser beam. With the power of 30 W was able to reach maximum temperature of 399 K at 120s and a distribution of a temperature sufficient to allow healing of the pHEMA hydrogel, using an infrared laser, for biomedical applications. Furthermore, it was observed that the effect of convection on the system can be neglected, since it presented little influence in the heating process of HEMA solutions.

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