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MATHEMATICAL MODELLING OF ONE DIMENSIONAL TEMPERATURE DISTRIBUTION AS A FUNCTION OF LASER INTENSITY ON CARBON FIBER REINFORCED POLY(ETHER-ETHER-KETONE)-(PEEK) COMPOSITE

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Abstract. Poly(ether-ether-ketone) (PEEK) is used in many area especially structural and industrial applications due to it has superior mechanical, chemical and thermal properties. Besides excellent electrical and thermal properties, carbon fibres have high specific tensile modulus and strength. Due to these properties, carbon fibers are frequently used as reinforcement materials in polymer matrices. While the polymer matrix determines the long-term durability of the composite system, light carbon fibers ensure that the material is durable and lightweight. Since composites have more than one materials together which are different thermal and mechanical properties, machining of composites is more complex than pure materials. Lasers are used in many industrial and high technological area. In this study, proposed mathematical model has been applied on the cavity formation on PEEK composite by single laser pulse using Fourier method with homogenous approach. The effects of the laser energy on temperature distribution in PEEK composite was investigated and the numerical model was obtained.

Keywords: Mathematical modeling, Laser Ablation, PEEK Composite, Heat Distribution, Heat Affected Zone.

AMS Subject Classification: 93A30, 42A38.

1. Introduction

The composites comprise two or more materials [1,2]. These different materials contribute to the composite material with their superior properties. The materials that make up the composite material have different mechanical and thermal properties [3]. Therefore, although different materials impart superior properties to the composite material, it also makes it difficult to process the composite materials. Carbon Fiber Reinforced Composite materials consist of polymer matrix which allows to hold material together and Carbon Fiber which adds durability to the material [4]. In addition to excellent electrical and thermal properties, CFs have high tensile strength modules and durability [5]. As with

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other polymer based composite materials, Poly (ether-ether-ketone) (PEEK) is used in many fields due to its superior mechanical, chemical and thermal properties [1].

The mechanical and tribological properties of composite materials can be changed by mechanical or heat treatment on composite materials. Laser surface texture is also used in many areas for this purpose. Many experiments are required to obtain surface shapes with the desired geometry in laser surface texture. When conducting these tests, it should be taken into consideration that the composite material is composed of materials with different mechanical and thermal properties. In addition, the parameters used in laser material processing must be selected appropriately. As the number of trials increases, so does the time and cost. One of the best ways to save time and test costs is to do mathematical modeling.

In this study, the proposed mathematical model was applied with a single laser pulse using the Fourier method with a homogeneous approach on cavity formation in PEEK composite. The effects of laser energy on temperature distribution in PEEK composite were investigated and a numerical model was obtained.

Laser pulses with different energies were sent to the carbon fiber reinforced PEEK composite plaque with a thickness of 3 mm. Nd: YAG laser has a wavelength of 1064 nm and an average power of 600 Watt was used in the ablation process. Spot size (diameter) at the surface is 400 μm which is the minimum value of spot size. Pulse duration was selected as 6 ms, Pulse energies of laser are 0.1, 1, 2, 3, 4 J.

2. Heat Distribution in Material

Before creating a mathematical model, firstly the mechanism of laser-material interaction, and then the heat distribution mechanisms should be examined. If the laser beam sent to the material has the required wavelength and sufficient energy, the molecules or atoms of the material begin to vibrate. This mechanical energy, which consists of vibrations, is converted into heat energy very quickly (10^{-12} to 10^{-6} s for nonmetals). Heat transfers in three ways: conduction in the material, convection and radiation from the surface.

To obtain the heat distribution equation, the solution of the one-dimensional heat conduction equation is necessary. Some assumptions should be made to simplify the solution. The material is assumed to be homogeneous in the direction of the fibers. The heat transfer rate is constant during the pulse duration (6ms). The heat transfers with convection and radiation have been ignored.

Temperature distribution equation for one-dimension can be obtained from the equation given below.

$$\frac{\partial T(z,t)}{\partial t} = \alpha^2 \frac{\partial^2 T(z,t)}{\partial z^2}, \tag{1}$$

where;
T: temperature as a function of time and position.,
α is the thermal diffusivity,
Thermal diffusivity can be described as below.

$$\alpha^2 = \frac{k}{c\rho}$$

, where,
k: the heat conduction coefficient,
c: ispecific heat,
ρ: density.
Let $t_p > 0$ be a fixed number and denote by $D = \{(z.t) : 0 < z < l, \ \ 0 \ < t < t_p\}$

where t_p is the pulse duration.
The initial condition can be written as;

$$T(z,0) = T_0, \quad 0 < z < l, \tag{2}$$

where T_0 is the initial constant temperature of the material (room temperature 20 C°).

The simple boundary condition at the surface (z=0) assuming that laser energy absorbed at the surface equals the energy conducted can be written as:

$$\frac{\partial T(0,t)}{\partial t} = 0, \frac{\partial T(l,t)}{\partial t} = 0 \qquad (t > 0). \tag{3}$$

This problem will be called a parabolic problem where $T(z,t) \in C^{2,1}(D) \cap C^{1,0}(D)$ is called classical solution of the problem (1)-(3). The problem of finding the heat source in a parabolic equation has been investigated in many studies [6, 7, 8, 9].

By applying the standard procedure of the Fourier method, we obtain the following representation for the solution of (1)-(3).

$$T(z,t) = Z(z)T(t)$$

$$\frac{Z''(z)}{Z(z)} = \frac{T'(t)}{\alpha^2 T(t)} = -\lambda^2,$$

where λ is fix number.

$$Z''(z) + \lambda^2 Z(z) = 0$$
$$Z'(0) = 0$$
$$Z'(l) = 0.$$

The solution of the last problem

$$Z(z) = C_{1k} cosmz + C_{2k} sinmz$$
$$Z'(z) = -mC_{1k} sinmz + mC_{2k} cosmz$$
$$C_{1k} = C_{1k} cosml + C_{2k} sinml$$
$$C_{1k} = -C_{1k} sinml + C_{2k} cosml$$
$$\begin{vmatrix} 1 - cosml & -sinml \\ sinml & 1 - cosml \end{vmatrix} = 0.$$

The eigenvalues are

$$_k = \left(\frac{2\pi k}{l}\right)^2, k = \overline{1,\infty}.$$

The eigienfunctions are

$$Z_1(z) = cos\frac{2\pi k}{l}z, \qquad Z_2(z) = sin\frac{2\pi k}{l}z$$

$$Z(z) = C_{1k} cos\frac{2\pi k}{l}z + C_{2k} sin\frac{2\pi k}{l}z$$

$$T'(t) + \alpha^2 T(t) = 0$$

$$\frac{dT}{T} = \alpha^2$$

$$T(t) = C_{3k} e^{-\left(\frac{2\pi\alpha k}{l}\right)^2 t}$$

$$T(z,t) = \sum_{k=1}^{\infty} \left(T_{ck} cos\frac{2\pi k}{l}z + T_{sk} sin\frac{2\pi k}{l}z\right) e^{-\left(\frac{2\pi\alpha k}{l}\right)^2 t}$$

$$T(z,0) = \sum_{k=1}^{\infty} \left(T_{ck} cos\frac{2\pi k}{l}z + T_{sk} sin\frac{2\pi k}{l}z\right).$$

Laser intensity varies through the material. Intensity can be found in any point by the Beer-Lambert's Law:

$$\frac{dI}{dz} = -aI.$$

It can be obtained after integrating the last equation.

$$\int_{I_0}^{I} \frac{dI}{I} = -\int_{b}^{z} adz$$

$$I = I_0 e^{-\int_b^z adz.} \tag{4}$$

When the thin film absorbs the laser beam energy, it generates heat. The heat generation rate is defined as,

$$S = -\frac{dI}{dz}. \tag{5}$$

Hence, the volumetric heat generation becomes:

$$S = I_o e^{-\int_b^z adz}. \tag{6}$$

When heat generation term is added to equation (1);

$$\frac{\partial T(z,t)}{\partial t} = \alpha^2 \frac{\partial^2 T(z,t)}{\partial z^2} + S(z,t) \tag{7}$$

with initial condition

$$T(z,0) = T_0, \quad 0 < z < l, \tag{8}$$

the boundary condition is

$$\frac{\partial T(0,t)}{\partial z} = 0, \frac{\partial T(l,t)}{\partial z} = 0 \qquad (t > 0). \tag{9}$$

We look for the following representation for the solution of (7)-(9);

$$T(z,t) = \sum_{k=1}^{\infty} \left(T_{ck} cos \frac{2\pi k}{l} z + T_{sk} sin \frac{2\pi k}{l} z \right). \tag{10}$$

By applying the Fourier method,

$$S(z,t) = \sum_{k=1}^{\infty} \left(T'_{ck}(t) cos \frac{2\pi k}{l} z + T'_{sk}(t) sin \frac{2\pi k}{l} z \right) + \alpha^2 \sum_{k=1}^{\infty} \left(\frac{2\pi k}{l} \right)^2 \left(T_{ck}(t) cos \frac{2\pi k}{l} z + T_{sk}(t) sin \frac{2\pi k}{l} z \right).$$

If we multiply both sides by

$$\int_0^l cos \frac{2\pi k}{l} zdz$$

$$T'_{ck}(t) + \left(\frac{2\pi k}{l} \right)^2 T'_{ck}(t) = S_{ck}.$$

The last equation is called as linear equation

$$S_{ck} = \int_0^l S(z,t) \, cos \frac{2\pi k}{l} dz$$

$$= e^{\int \left(\frac{2\pi k}{l} \right)^2 dt} = e^{\left(\frac{2\pi k}{l} \right)^2 t}$$

$$T_{ck}(t) \, e^{\left(\frac{2\pi k}{l} \right)^2 t} = \int_0^t S_{ck} e^{-\left(\frac{2\pi k}{l} \right)^2 \tau} d\tau + \varphi_{ck}$$

$$T_{ck}(t) = \int_0^t S_{ck} e^{-\left(\frac{2\pi k}{l} \right)^2 (t-\tau)} d\tau + \varphi_{ck} e^{-\left(\frac{2\pi k}{l} \right)^2 t}.$$

With same estimations, we obtain

$$T_{sk}\left(t\right)=\int_0^t S_{sk}e^{-\left(\frac{2\pi k}{l}\right)^2(t-\tau)}d\tau+\varphi_{sk}e^{-\left(\frac{2\pi k}{l}\right)^2 t}.$$

We obtain the following representation for the solution of (7)-(9);

$$T\left(z,t\right)=\sum_{k=1}^{\infty}\left(\varphi_{ck}e^{-\left(\frac{2\pi k}{l}\right)^2 t}+\int_0^t S_{ck}(z)e^{-\left(\frac{2\pi k}{l}\right)^2(t-\tau)}d\tau\right)cos\frac{2\pi k}{l}z$$

$$+\sum_{k=1}^{\infty}\left(\varphi_{sk}e^{-\left(\frac{2\pi k}{l}\right)^2 t}+\int_0^t S_{sk}(z)e^{-\left(\frac{2\pi k}{l}\right)^2(t-\tau)}d\tau\right)sin\frac{2\pi k}{l}z$$

$$T\left(z,t\right)=\sum_{k=1}^{\infty}\left(\varphi_{ck}e^{-\left(\frac{2\pi k}{l}\right)^2 t}+\int_0^t\int_0^l S\left(z,t\right)cos\frac{2\pi k}{l}e^{-\left(\frac{2\pi k}{l}\right)^2(t-\tau)}dzd\tau\right)cos\frac{2\pi k}{l}z$$

$$+\sum_{k=1}^{\infty}\left(\varphi_{sk}e^{-\left(\frac{2\pi k}{l}\right)^2 t}+\int_0^t\int_0^l S\left(z,t\right)cos\frac{2\pi k}{l}e^{-\left(\frac{2\pi k}{l}\right)^2(t-\tau)}dzd\tau\right)sin\frac{2\pi k}{l}z. \qquad (11)$$

3. Application of the Model

In our study, the simple boundary condition at the surface (z=0) assuming that laser energy absorbed at the surface equals the energy conducted can be written as:

$$-k\frac{\partial T(0,t)}{\partial z}=H$$

where k is the thermal conductivity and H is the absorbed laser energy. The absorbed laser energy H can be given by the product of absorptivity A and incident laser power density I_0 (i.e., $H=AI_0$). If t_p is the irradiation time (pulse on time) then the parameter equals unity when the laser is on, i.e., $0\le t\le t_p$. It can be taken as zero when the laser is off, i.e., $t>t_p$.

$$\frac{\partial T(z,t)}{\partial t}=\alpha^2\frac{\partial^2 T(z,t)}{\partial z^2}+S(z,t) \qquad (12)$$

with initial condition

$$T\left(z,0\right)=T_0,\quad 0<z<l \qquad (13)$$

the boundary condition is;

$$\frac{\partial T(0,t)}{\partial z}=0,\frac{\partial T(l,t)}{\partial z}=-\frac{H}{k}\qquad\left(t>0\right). \qquad (14)$$

The solutions of these equations can be obtained as follows:
During heating ($0<t<t_p$):

$$T\left(z,t\right)=\sum_{k=1}^{\infty}\left(\varphi_{ck}e^{-\left(\frac{2\pi\alpha k}{l}\right)^2 t}+\int_0^t\int_0^l S(z,t)cos\frac{2\pi k}{l}ze^{-\left(\frac{2\pi\alpha k}{l}\right)^2(t-\tau)}dzd\tau\right)cos\frac{2\pi k}{l}z$$

$$+\sum_{k=1}^{\infty}\left(\varphi_{sk}e^{-\left(\frac{2\pi\alpha k}{l}\right)^2 t}+\int_0^t\int_0^l S(z,t)cos\frac{2\pi k}{l}ze^{-\left(\frac{2\pi\alpha k}{l}\right)^2(t-\tau)}dzd\tau\right)sin\frac{2\pi k}{l}z-\frac{zH}{lk}. \qquad (15)$$

4. Numerical Solution

Heat equation is solved numerically using the finite difference method.Implicit scheme is used for this work. We subdivide the intervals [0,1] and [0,T] into subintervals N_x and N_t of equal lengths $h = \frac{\pi}{N_x}$, $\tau = \frac{T}{N_x}$, respectively. We choose the implicit scheme which is absolutely stable and has a second-order accuracy in h and a first-order accuracy in τ. The implicit scheme for (12)-(14) is as follows:

$$\frac{1}{\tau}\left(T_i^{j+1} - T_i^j\right) = \frac{1}{2h^2}\left(T_{i-1}^{j+1} - 2T_i^{j-1} + T_{i+1}^{j+1}\right) + S_i^j. \tag{16}$$

$$T_i^0 = T_i. \tag{17}$$

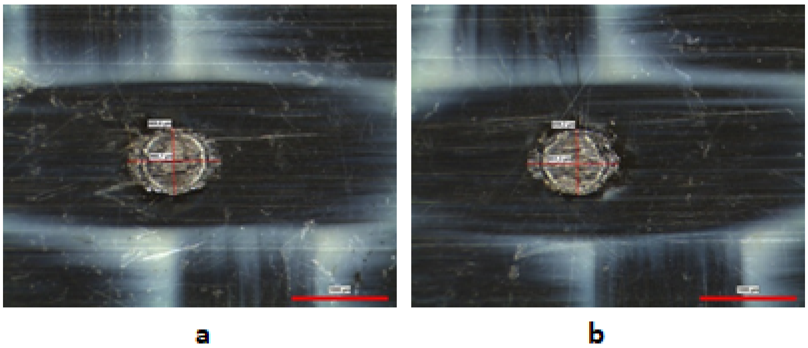
$$T_0^j = T_{N_{x+1}}^j.$$

$$\frac{T_1^j + T_{N_{x+1}}^j}{2} = T_{N_{x+1}}^j \tag{18}$$

where $i \in [0,1]$, $j \in [0,\mathrm{T}]$ are the indices for the spatial and time steps respectively, at the level t=0, adjustment should be made according to the initial condition and the compatibility requirements. The system of equations (16)-(18) can be solved by the Gauss elimination method and T_i^{j+1} is determined. If the difference of values between two iterations reaches the prescribed tolerance, the iteration is stopped and we accept the corresponding values T_i^{j+1}on the (j+1)-th time step.

5. RESULTS AND DISCUSSION

To reduce the error rate, each trial was performed twice. The optical microscope image of the obtained cavities was shown in Fig. 1. Boundaries of melting and vaporization region were measured with Fig. 1. Cavities shown in Fig. 1a and Fig. 1b were obtained by single laser pulse with 0.1 J pulse energy. Cavities shown in Fig. 1c and Fig. 1d were obtained by single laser pulse with 1 J pulse energy. Cavities shown in Fig. 1e and Fig. 1f were obtained by single laser pulse with 2 J pulse energy. Cavities shown in Fig. 1g and Fig. 1h were obtained by single laser pulse with 3 J pulse energy. Cavities shown in Fig. 1i and Fig. 1j were obtained by single laser pulse with 4 J pulse energy. All pulses have 2 ms pulse durations. Heat Affected Zone limits were measured at the point where the polymer matrix didn't melt. Measured values of HAZ limits were given in Table 1.



a b

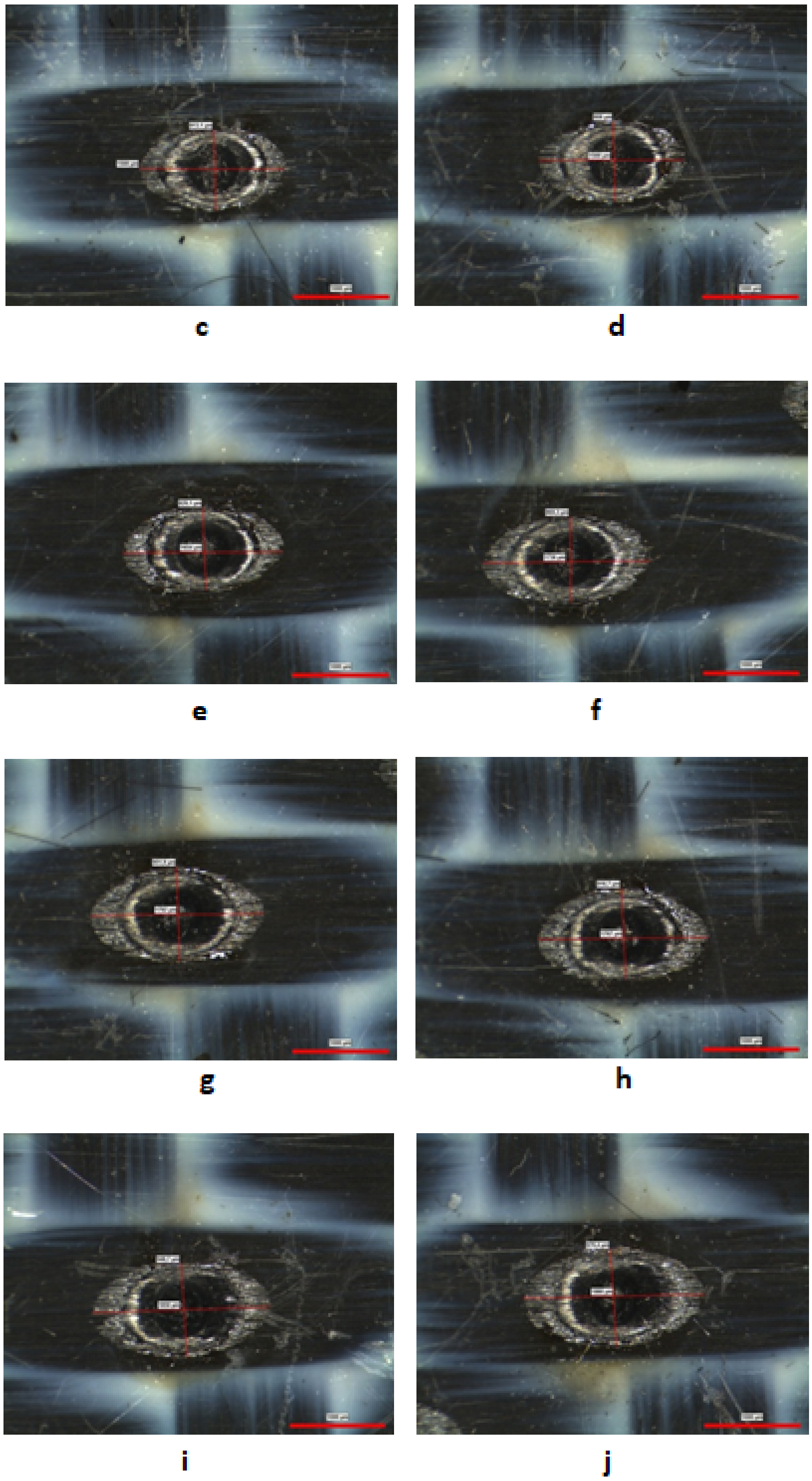


FIGURE 1. Optical microscope images of cavities obtained with (a) and (b) 0.1 J pulse energy, (c) and (d) 1 J pulse energy, (e) and (f) 2 J pulse energy, (g) and (h) 3 J pulse energy, (i) and (j) 4 J pulse energy.

Energy (j)	Laser Intensity (W/m^2)	Mean HAZ size (µm)
0.1	0.8×10^8	959
1	7.96×10^8	1500
2	15.92×10^8	1695
3	23.89×10^8	1780
4	31.85×10^8	1865

Table 1. Applied laser energy and HAZ diameter measured from images.

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