Mathematical Modelling Time Dependent for Heat Transfer Process in Homogenous Composite ZnO/Activated CNF

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Abstract. A theoretical study of heat transfer on composite Zinc Oxide (ZnO)/Activated Carbon Nanofibers (CNF) by using mathematical model from diffusion equation for stationary composite with various heating time was studied. The equation and boundary conditions are interpreted by using Taylor series expansion to obtain a steady-state numerical solution from the Jacobi iteration algorithm. The composites were put inside the furnace model by filaments on the two sides of the walls as the source of heat (general model for furnace). By using this model, the position of sample to receive the homogeneous temperature determined. We compared the steady-state and unsteady-state conditions to identify the temperature distribution at real-time. The results show that the heat distribution will reach an asymptotic state by performing a numerical analysis is 200 K and 300 K for 25 minute time of heating. In this study, shows the efficient way for annealing homogenous materials to identify the position inside the furnace which can be used as a guide to receive the homogenous temperature during the annealing processes.

1. Introduction
Treatment of materials during and or post growth by annealing processes is used to identify the temperature stability of the materials which is the key factor in device applications and performance. Annealing processes at high temperatures usually used in industrial production and also for research in laboratory scale. Recently, there are many scientific reported that the composite of ZnO/CNF (carbon nanofibers) used annealing treatment for production of carbon nanofibre as well as in composite form which are candidate materials for supercapacitor electrodes [1]. Carbon nanofibers (CNF) are carbon material with interconnected three-dimensional mesoporous texture and very good thermal stability which was promising electrode material for supercapacitors [2-10]. The temperature of annealing is the important parameter was strongly influenced to the properties such as surface area, pore size and
distributions, which play an important role in the performance of electrochemical capacitance [8-21]. The sample position inside the furnace is the key factor in receiving the homogenous temperature of the sample in laboratory scale as well as also in the industrial production.

Therefore, in this paper, a theoretical approach was used to describe the temperature distribution of composites ZnO/activated CNF by using diffusion equations. The assumption of the composite ZnO/CNF is homogeneous particles and the distribution is uniform. The purpose in this study is to establish a mathematical model which is suitable for the distribution temperature in the furnaces by determining the optimal conditions of the system. The effects of continuous annealing are producing the heat conduction distribution in the system and also the convection flows from material to air due to the system is un-isolated from the environment. The heat transfer processes during the annealing in the furnace model will be analyzed by numerical system.

2. Mathematical Model for ZnO/CNF Composite Heating Process

2.1 Model and Assumption

In this paper, we describe the annealing model of homogenous material in the furnace with filaments as heating sources continuously propagate conduction to the composite ZnO/CNF. We assumed that in the heating processes there no gap between the filament and the material, so there is no difference in thermal conductivity distribution in the ZnO/CNF composite.

![Figure 1. Modeling of gas-solid heat transfer in ZnO/CNF for homogeneous composite](image)

In this study, the furnace filaments are placed at the top ($T_{11}$) and at the bottom ($T_{00}$) of the composite ZnO/CNF. While the right and left sides of the material are un-isolated, so there is a heat exchange between material and air, we assumed that the cooling process in the gas-solid phase. The cooling process is characterized by the presence of a convection flow coefficient ($h$) from the material into the air. By this assumption, the heating process is described in 2-dimensional coordinate with length $A$ and width $B$ for the stationary system as can be in Figure 1.

2.2 Mathematical Description of Heat Transfer Process

In this case, a mathematical equation is needed for represents the temperature distribution in the material. For this reason, the diffusion equation can represent the state of the case by the second-order differential equation in 2-dimensional form. The diffusion equation is expressed by:

$$\rho C_p \left( \frac{\partial T}{\partial t} \right) = \lambda \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$  \hspace{1cm} (1)

The form of the equation in the left side is the temperature variation of the composite ZnO/CNF with a certain time and in the right side are heat diffusion processes in the composite.
In the stationary state, there is a heat exchange between composite ZnO/CNF with the environment due to both sides of the furnace model is un-isolated which was allows the convective heat transfer. Assuming the gas-solid phase heat coefficient is \( h \) and certain surface area is \( a \), then the amount of convective heat transfer can be calculated by using the equation \( ha(T_2 - T_1) \), where \( T_2 \) is the temperature in the material, while \( T_1 \) is the temperature at a boundary between material and the environment. By considering the conduction heat transfer accompanied by convection, the equation (1) becomes the equation (2) as follows:

\[
\rho C_p \left( \frac{\partial T}{\partial t} \right) = \lambda \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - ha(T_2 - T_1)
\]

(2)

The \( C_p \) is heat capacity; \( \rho \) is the density; \( \lambda \) is the thermal conductivity of the composite.

By using the first thermodynamic law for the gas-solid phase, the equation (2) can be solved using the Finite Element Method (FEM). The sources of heat are filaments located at the top and the bottom of composite with continue warm up and heating to the desired temperature.

In the heat transfer simulations that are accompanied by cooling, there are boundary conditions for finding analytical solutions according to the assumption of the model. At the top and bottom, there is a continuous heat source of magnitude \( T_{00} \) and \( T_{11} \). For the right and left position, there is the heat exchange between the material and the environment. The boundary conditions can be written as follows;

\[
\begin{align*}
T(x, B) &= T_{11} ; 0 < x < A \\
T(x, 0) &= T_{00} ; 0 < y < B \\
\frac{\partial T}{\partial y}(0, B) &= T_{22} \\
\frac{\partial T}{\partial x}(A, y) &= 0
\end{align*}
\]

(3)

From the boundary conditions applied to the heating system, we can analyze by using the numerical solutions.

2.3 Discretization of Differential Equations and Boundary Conditions

The numerical methods used to solve differential equation solutions with certain boundary conditions are by using finite element method. The first is determining domain which can be represented by the global matrix. Furthermore, domain is discretized by dots to form a rectangular which called a grid. These points are represented by the local matrix for determine domain of heat properties. So that material domain is a set of grids that called mesh as can be seen in Figure 2.
For example, the domain of material consisting of 50 x 100 grids, representation of the domain is illustrated by the global matrix as shown in Figure 3a and 3b. For illustration of one element is representation by a local matrix as shown in Figure 3c, which is for each corner filled by local number points of each element.

After discretizing the domain, a trial function is obtained by:

$$T(x,t) = N_1(x)T_1(t) + N_2(x)T_2(t) + \cdots$$ (4)

where $N(x)$ is an interpolation function at the four vertices as expressed:

$$N_1(r,s) = \frac{1}{4}(1 - r)(1 - s) \quad N_3(r,s) = \frac{1}{4}(1 + r)(1 + s)$$

$$N_2(r,s) = \frac{1}{4}(1 + r)(1 + s) \quad N_4(r,s) = \frac{1}{4}(1 - r)(1 + s)$$

The obtained trial function was included in the control differential equation by using Jacobian iterations. It was found that, the heat distribution in each grid changes by the increasing time of annealing.

2.4 Flow Chart for Numerical Solution

The flow chart for numerical solutions in this study with differential equation as shown in fig. 4 as follows ;
3. **Result and Discussion**

This model uses Jacobian iteration to solve the solution of the differential diffusion equation. The software used is Scilab 6.0.1 from Scilab Enterprises to determine and check the solution is converged or not. The maximum absolute error of two successive iterations must be below the threshold $10^{-4}$ [22].
Figure 5. State of the plate at the initial temperature (room temperature) (a) $\delta = 0.167 \text{ cm}$ dan (b) $\delta = 0.125 \text{ cm}$. Heat distribution asymptotically (c) $\delta = 0.167 \text{ cm}$ dan (d) $\delta = 0.125 \text{ cm}$. Heat distribution at steady state (e) $\delta = 0.167 \text{ cm}$ dan (f) $\delta = 0.125 \text{ cm}$.

Fig. 5 clearly shows the distribution of temperature for the homogeneous sample inside the furnace. The position of the sample in every condition (from initial to steady state) should be in the middle of the furnace to receive the homogenous temperature during annealing processes.

3.1. Verification in grid arrangement
In the boundary element method, the matrix representation as the domain form which was described the heat distribution for each grid. In this study, the grid arrangement is very
important to determine the accuracy of the numerical solutions obtained. The accuracy of the solutions indicated by the number of grids, for high number the solutions are more accurate and approaching the exact solution [22].

For validation in this simulation, the domain of the ZnO/CNF composite is arranged for length and width is 1 cm. Grid were settings by given with variations are 0.167 cm and 0.125 cm with the time iteration for each grid is 2000 steps. The heat distribution for each grid is presented in Figure 3. The solution that approached accuracy results with the numerical solution is for grid 0.125 cm as similar reported in Ref. [22].

3.2. Numerical Analysis for ZnO/CNF Plate Composite Heating Process

Numerical analysis of a differential equation is very important for the accuracy of the solutions obtained. The key point in the numerical analysis is the condition of convergence and stability of asymptotic values. A mathematical model approaches the exact value when the model satisfies the convergence condition. This means that the variations of annealing temperature depend on the grid and the asymptotic state will converge at one particular point. The asymptotic state is constant indicated that the stable value of annealing temperature. In this study shows the asymptotic state for the threshold below 10^{-4} is at 25 minute and the temperature at 200 K and 300 K.

Figure 6 shows the left side reduce temperature probably due to the exchange of temperature with air by the convection process and the conduction process in the materials. The effective heat transfer coefficient between conduction process and the convection by the air is calculated by using:

\[ k = \frac{1}{\ln \left( \frac{r}{\phi} \right)} \]  

where \( r \) is the radius of particle; \( \phi \) is the composite correction factor, equal 0.25.

Figure 7 shows comparison between the steady-state and unsteady-state to the y-axis discretization point. The error value for the steady-state and unsteady-state conditions for the grid 0.125 cm is smaller than that of the grid 0.167 cm due to the accuracy solution from FEM is in terms of convergence the number of grids. There are two methods for accurate solution approaches is h-refinement which is refers to the process of increasing the number of elements used in the model of particular domain and reduce the size of individual elements. For the
second method is \emph{p-refinement} which is emphasizes in the increasing the order of polynomials for an interpolation function [23].

![Figure 7](image_url)

\textbf{Figure 7.} Comparison of steady-state and unsteady-state states at the y-axis discretization point (a) $\delta = 0.167$ cm (b) $\delta = 0.125$ cm.

4. Conclusion

A mathematical model for annealing homogenous composite ZnO/CNF is based on the diffusion differential equations for steady-state conditions and dependent on time for stationary domain systems. Numerical solutions for the temperature distribution were obtained by using the finite element method (FEM) which is approach to the exact solution. The solutions can be seen in terms of convergence and stability of the asymptotic values which were analyzed by numerical systems. The efficiency of the annealing system obtained for the asymptotic state is in step 1500 for all grids. Thus, the effective time for annealing composite ZnO/CNF to receive homogenous temperature is 25 minute with a temperature at 200 K and 300 K. The position of the sample in every condition (from initial to steady state) should be in the middle of the furnace to receive the homogenous temperature during annealing processes.

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