NANO ENGINEERED FIRE RESISTANT COMPOSITE FIBERS (M02-D08)

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Objective:

In the first part, the heat transfer behavior of particle reinforced nanofibers is discussed and compared with the conventional concepts. The interface as a barrier is analyzed. The material consists of cylindrical disks embedded into nanofibers with cylindrical shape. We used the thermal resistance method to analyze the effect of barrier. The second part consists of manufacturing. A novel method is introduced to gather the nanofiber to form yarn.
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Key words: nanofibers, heat transfer coefficient, interface, thermal resistance and FEM.

Nomenclatures	**Subscripts**	**Greeks**
k thermal conductivity	+ dimensionless	β k_d/k_b
l length	**b** barrier	γ k_b/k_f
Q heat flow rate	**d** disk (particle)	
r radius	**ef** effective	
v volume fraction	**f** fiber	
t thickness of the interface	λ dimensionless heat transfer coefficient	
R thermal resistance	**1,2,3** domains	

Introduction:

Thermal conductivity is important to define flammability properties. A recent study done by Kashiwagi et al., shows that, by measuring thermal properties, we can understand the flammability properties [1]. Heat transfer takes place when there is a temperature difference in the material, and heat is transferred by conduction, convection or radiation. When the size of the material decreases, the importance of the molecular behavior becomes much higher, the free path plays an important role, and the conventional belief of heat transfer disappears.

In nanoscale, the thermal conductivity of homogeneous material can be calculated by three different techniques of molecular dynamics. (1) Equilibrium molecular dynamics with the Green-Kubo's formula, (2) Non-equilibrium molecular dynamics (NEMD) developed by Evens and (3) Non-equilibrium molecular dynamics with direct temperature differences [2]. Cahill et al. critically reviewed the studies about the thermal transport in nanostructures. Although this work focused on electronic devices, it gives a brief understanding about thermal transport [3]. Mirmira et al. summarized the studies related to thermal conductivity of thin films in nano scale[4]. There are many thermal conductivity models for thin films. [5]. Berber et al combined the equilibrium and non equilibrium molecular dynamic simulations and found a thermal conductivity of a 6600 W/mK, which is unusual [6].

In macro modeling, many researchers have discussed heat behavior either by using analytical [7] or numerical modeling [8]. Springer and Tsai used a theoretical approach to find out the transverse thermal conductivity by using shear loading analogy and square packing array [9]. In another analytical study, Rayleigh and Maxwell's theories were modified by Hasselman and Johnson [10]. In their approach, they assumed a continuous behavior and derived relations for a single coated fiber which is surrounded by matrix. There is no experimental comparison of these approaches.

One of the important factors to understand the difference between nano and macro structures is interface effect. To support this, it is necessary to obtain either experimental or simulation results. It seems from the studies that much of the information could be gathered from the simulations because of the lack of analytical calculations. There is still no clear explanation to make the interface clear in minds. What do we see at the interface? What kind of bonding could appear? What kind of topology, transport across it, deformation, chemical activities, and forces also could appear?
Van Assche and Van Mele discussed the effect of the interphase. They emphasized that macroscopic proporties of composite materials, including fiber-reinforced polymers, blends, and multilayer systems, were often strongly affected by the develepment of interphase regions with properties differing from the properties of the constituent materials. Interphases could arise due to

preferential adsorption, catalytic influences of a surface, inter-diffusion, phase separation, etc. The resulting gradients in composition (polymer blends) or crosslink density (thermosets) lead to graidents in the microscopic properties[11]

Modeling by using Thermal Resistance Method:

In analytical modeling, we modified the method developed by Zou, Yu and Zhang [12]. They used an electrical analogy technique and modeled the cylindrical filament-square packing array unit cell to find out the transverse thermal conductivities (Figure 1).

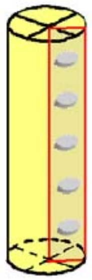	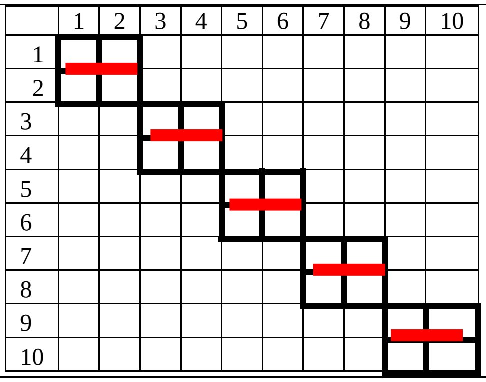	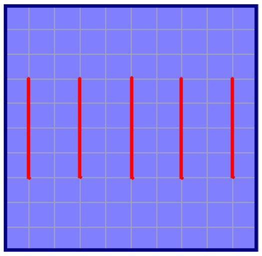	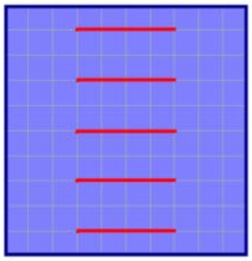
Main model	Dividing the model into symmetry parts.	Fiber distribution with a ratio of 4-5%; vertical.	Fiber distribution with a ratio of 4-5%; horizontal.

Figure 1. Initial modeling steps.

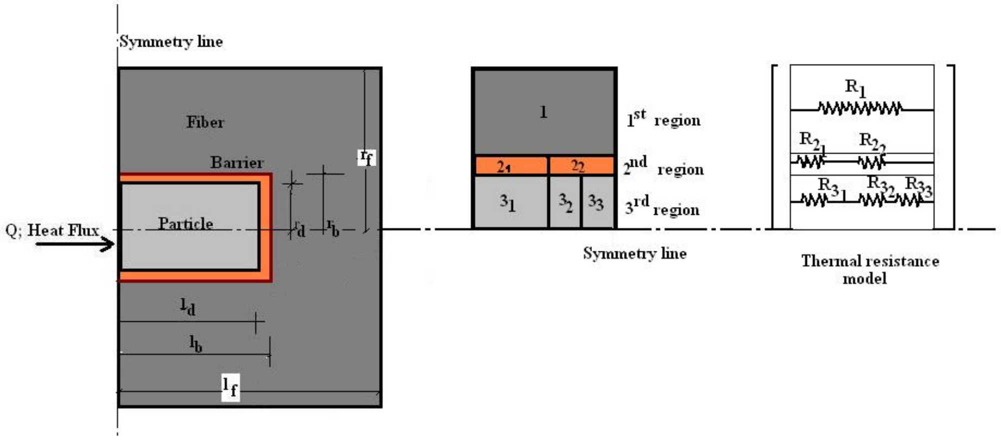

Figure 2. Analytical modeling of particle reinforced nanofibers.

Basically, there are three components in the model; fiber, barrier and particle (Figure 2). In the first region, only fiber appears, in the second region, there is a fiber and a barrier and in the third region all three components exist. This can be seen from the equations given below;

First region;	Second region;

$$R_1 = \frac{l_f}{k_f(r_f - r_b)} \qquad R_2 = R_{2_1} + R_{2_2} = \frac{l_b}{k_b(r_b - r_d)} + \frac{(l_f - l}{k_f(r_b -}$$

(1)

Third region;

$$R_3 = R_{3_1} + R_{3_2} + R_{3_1} = \frac{l_d}{k_d r_d} + \frac{(l_b - l_d)}{k_b r_d} + \frac{(l_f - l_b)}{k_f r_d}$$

Total thermal resistance;

$$\frac{1}{R_{total}} = k_{ef} = \frac{1}{R_1} + \frac{1}{R_2} + \frac{1}{R_3} = \frac{k_f(r_f - r_b)}{l_f} + \frac{1}{\frac{l_b}{k_b(r_b - r_d)} + \frac{(l_f - l_b)}{k_f(r_b - r_d)}} + \frac{1}{\frac{l_d}{k_d r_d} + \frac{(l_b - l_d)}{k_b r_d} + \frac{(l_f -}{k_f r}}$$

Effective thermal conductivity ratio is given by;

$$k_{ef} = \frac{k_f(r_f - r_b)}{l_f} + \frac{k_b k_f((r_b - r_d))}{l_b k_f + k_b(l_f - l_b)} + \frac{k_d k_b k_f r_d}{l_d k_b k_f + (l_b - l_d)k_d k_f + (l_f - l_b)k_d k_b} \tag{5}$$

In order to make the formula dimensionless, let;

$$\beta = \frac{k_d}{k_f} = \quad \gamma = \frac{k_b}{k_f} \quad b = \frac{r_f}{r_b} \quad \nu_d = \frac{r_d l_d}{r_f l_f} \quad \nu_b = \frac{r_b l_b}{r_f l_f} \quad \frac{\nu_d}{\nu_b} = \frac{r_d l_d}{r_b l_b}$$

$$t = r_b - r_d \quad t^+ = \frac{t}{r_d} = \frac{r_b}{r_d} - 1 \quad \lambda = \frac{h_b r_d}{k_f} \quad h_b = \frac{k_b}{t}$$

$$\nu_b = \frac{r_b l_b}{r_f l_f} \rightarrow \nu_b b = \frac{l_b}{l_f} \rightarrow \nu_b b = \frac{l_b}{r_f} \tag{6}$$

$$b = \frac{r_f}{r_b}$$

and also let;

$$l_f = r_f \quad l_d = \frac{1}{10} r_d \quad t = \frac{1}{100} r_d \tag{7}$$

Then by using dimensionless variables,

$$k^+ = \frac{k_{ef}}{k_f} = 1 - \frac{1}{b} + \frac{\gamma}{11 + 101\gamma b - 11\gamma} + \frac{100\gamma\beta}{10\gamma + \beta + (101b - 11)\gamma\beta} \tag{8}$$

If the barrier thickness is taken as zero, some of the dimensionless variables and the final formula will become;

$$\gamma = \frac{k_b}{k_f} = \frac{k_f}{k_f} = 1 \quad b = \frac{r_f}{r_b} = \frac{r_f}{r_d} = \sqrt{\frac{1}{10V_d}} \tag{9}$$

$$\boxed{k^+ = 1 - \frac{100}{101}\sqrt{10V_d} + \frac{100\beta}{10 + \beta + \left(101\sqrt{\frac{1}{10V_d}} - 11\right)\beta}} \tag{10}$$

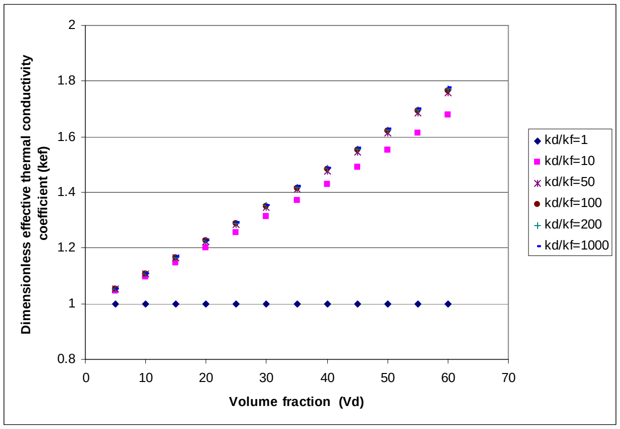

Figure 3. Effective thermal conductivity by using thermal resistance model

When the effect of volume fraction on thermal conductivities is compared in Maxwell and Lewis-Nielsen models, it is seen that Lewis- Nielsen method gives more accurate results when the filler ratio increases in the composite. Our model gave almost a linear relationship compared to the other models.

Computer Modeling

The problem consists of two substances: the fiber and the particle. Both of them have their thermal conductivity coefficients and so the aim is to get an efficient thermal conductivity coefficient. In order to avoid nano size effect and to provide a continuous modeling, we choose the size that finite element analysis can be applied.

In modelling part, we compared analytical and finite element models. Finite element modelling was done by using ANSYS7.0. As the element type, we used SOLID90 which allows us to model cylindrical shape. The constant heat flux was applied as 50 kW/m^2. Meshing was done automatically and the symmetry was used to avoid memory effect (Figure 4).

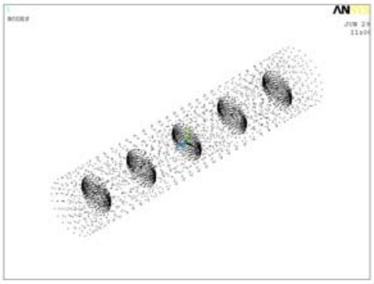	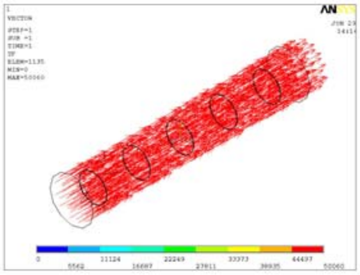	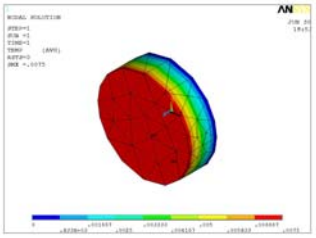
ANSYS model	Heat flux variation	Temperature distribution in symmetry part

Figure 4. The heat conduction model.

Manufacturing:

The continuous nanofiber based yarn manufacturing is a challenge. We need to have controlled voltage distribution and also need to get optimum viscosity in the solution. Beside this, one of the problems is alignments. One method is to use a rotating collector or to use a thin wheel with sharp edge. A possible nanofiber web collecting mechanism is shown in Figure 5.

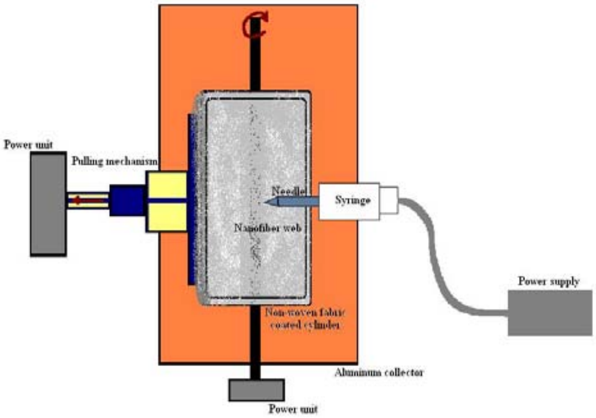

Figure 5. Experimental device

The device consists of:

- Basic electrospinning device
    - Needle and syringe
    - Power supply
    - Pressure device for giving stable solution flow.
- Pulling mechanism which forwards the gathered nanofiber web to the next process.
- Non woven fabric covered cylinder which must have a conductor made of aluminum and this part must be attached to the main collector to gather the nanofibers.
- Mechanicsms to give the desired movement for both cylinder **(↲ /↨)** and pulling mechanism **(←/→)**.

Activities:

Publications/Presentations:

1. Adanur, S., and Ascioglu, B., “Nanocomposite Fiber Based Web and Membrane Formation and Characterization”, Journal of Industrial Textiles, Vol. 36, No. 4, April 2007, pp. 311-327.
2. Ascioglu B., and Adanur, S., “Heat Transfer Behavior of Particle Reinforced Composites”, Developments in Theoretical and Applied Mechanics, Vol. **22**, Tuskegee-AL, 572-578 (2004).
3. Ascioglu, B., and Adanur, S., “Heat Transfer Modeling of Nanofiber Reinforced Composites”, Auburn University Annual Research Forum, Auburn, AL, March 2004.
4. Adanur, S., Ascioglu, B., “Processing Characterization of PVA Nanofibers in Electrospinning”, ICCE-11, Hilton Head, SC, August 8-14, 2004.

5. Ascioglu, B., Adanur, S., "Modeling of Thermal Conductivity in Nanofiber reinforced composites", ICCE-11, Hilton Head, SC, August 8-14, 2004.

Industry contacts:

Dr. Adanur and Ms. Ascioglu visited the Twitchell Company, Dothan, AL, in August, 2004. Twitchell is interested in coating the yarns with nanofibers for dyeing purposes.

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