

# Mathematical modeling of the fracture toughness of phenol formaldehyde composites reinforced with E-spheres

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**Abstract.** The fracture toughness of SLG filled phenolic composites have been determined by short bar tests. It is expensive to prepare the samples for the tests. Therefore, it is necessary to develop a mathematical model that will predict the fracture toughness of particulate filled phenolic composites. Mathematical models for tensile strength, Young's modulus are available but not for impact strength and fracture toughness. There is no sign that it can be built up from simple mathematical model; polynomial interpolation using Lagrange's method was therefore employed to generate the fracture toughness model using the data obtained from experiments. From experiments, it was found that the trend of the fracture toughness of the samples cured conventionally was similar to that cured in microwaves; it is therefore possible to predict the fracture toughness of the samples cured in microwaves from shifting the mathematical model generated for fracture toughness of samples post-cured in conventional oven. The shifted model represented the fracture toughness of the samples cured in microwaves very well.

## Introduction

Unlike the result of an impact test, it is a property that can be quantitatively measured. A typical fracture toughness test may be performed by applying a tensile stress to a specimen prepared with a flaw of known geometry and size. The stress applied to the material is intensified at the flaw [1]. For a simple test the stress intensity factor,

$$K = f\sigma \sqrt{\pi a} \quad (1)$$

The critical stress intensity factor is defined as fracture toughness,  $K_c$  is the  $K$  required for a crack to propagate and

$$K_c = f\sigma_c \sqrt{\pi a} \quad (2)$$

$K_c$  is a property that measures a material's resistance to brittle fracture when a crack is present and its unit is  $\text{MPa}\sqrt{m}$ . The value  $K_c$  for this thick-specimen situation is known as the plane strain fracture toughness  $K_{Ic}$ ; furthermore, it is also defined by [2].

$$K_{Ic} = f\sigma \sqrt{\pi a} \quad (3)$$

## Materials

The commercial resole resin used in the fracture toughness study was J2027 and manufactured by Borden Chemical Pty. Its official name is now Hexion Cellobond J2027L because the company had been taken by Hexion [3]. The acid catalyst used to crosslink the resin was Hexion Phencat 15 [4]. The ratio by weight of the resin to hardener for all samples in this work was chosen to be 50: 1. The polymer based on phenolic resin is Phenol-formaldehyde (PF). The PF resins are formed by the reaction of phenol with formaldehyde.

The Enviroshperes, E-spheres or SLG is a mineral additive that can improve product by reducing product's weight, improving its performance and lowering its cost. E-spheres are white microscopic hollow ceramic spheres that are ideal for a wide range of uses.

### Short Bar Test and Composite Samples

Baker described the background, selection criteria and specimen geometry options for short rod and short bar methods [5]. The background, selection criteria and specimen geometry options for the samples were clearly explained, which made the manufacture of the samples easier. The equation for fracture toughness in a short bar test can be derived from basic fracture mechanics using the assumptions of linear elastic fracture mechanics (LEFM). The requirements for LEFM were explained clearly, which were used in this study. The equation for the material plane strain critical stress intensity factor,  $K_{ICSB}$  [5]:

$$K_{ICSB} = \frac{(F_{max} Y_m^*)}{B\sqrt{W}} \quad (4)$$

$B = 50$  (by design), and  $F_{max} = 222$  N (average peak load of six samples, 222 N was used in the calculation of  $K_{ICSB}$ ). Fracture toughness for 20% by weight of SLG is calculated as:

$$K_{ICSB} = \frac{(F_{max} Y_m^*)}{B\sqrt{W}} = 8.800 \text{ MPa}\sqrt{m}$$

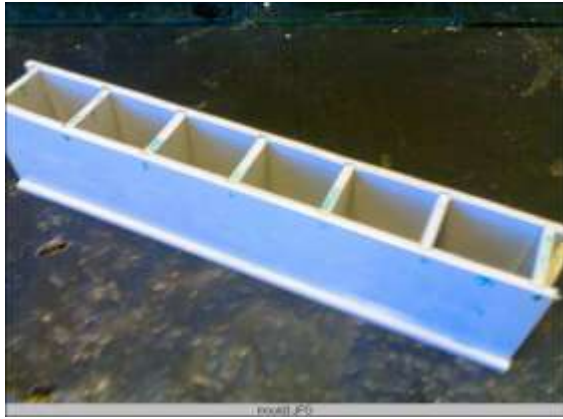
The reinforcer was SLG (ceramic hollow sphere) particulates and they were made 0 % to 35 % by weight in step of 5 % in the cured phenol formaldehyde composite PF/E-SPHERES (X %), where X is the percentage by weight of the filler; the 40% by weight was tried but it was found to be too viscous for mixing. As the raw materials of the composites are liquid and ceramic hollow spheres, the short bar specimens were cast to shape. The resin is mixed with the catalyst, after which the SLG is added to the mixture and they were then mixed to give the uncured composite. The mould was made from PVC (poly vinyl chloride) sheets with six pieces of short bar specimen each. This is depicted in Figure 1. The slots were made by inserting plastic sheets of suitable thickness. After preliminary curing, the samples were taken out of the mould and post-cured either in an oven at 50 °C for 4 hours followed by 80 °C for 4 hours and finally by 100 °C for 2 hours, or in microwaves by bringing the temperatures of the specimens to 100 °C using specified duration of exposure and power level and then cooled in the oven cavity. These specimens were then subjected to short bar test [6].

### Sample Size

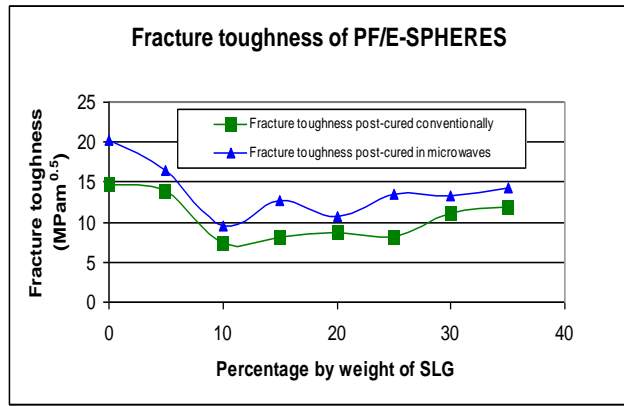
For each percentage by weight of SLG, there were two groups of six samples. One group was post-cured conventionally and the other was cured by microwave irradiation as described above. The short bar tests involve an opening load being applied near the mouth of the specimen, causing a crack to initiate at the point of the chevron slot. Figure 2 shows the fracture toughness of PF/E-SPHERES with varying percentage by weight of SLG.

### Mathematical modeling

Polynomial curve fitting technique was used to derive analytical terms that match given data points [7]. Polynomial curve fitting is a mathematical procedure for finding the best-fitting curve to a given set of points by minimizing the sum of the squares of the offsets of the points from the curve. More specifically, the Matlab function "Polyfit" was used to find the



**Figure 1: The mould for short bar specimens**



**Figure 2: Fracture toughness of PF/E-SPHERES with varying percentage by weight of SLG**

coefficients of a polynomial  $p(x)$  of degree  $n$  that fit the data,  $p(x(i))$  to  $y(i)$ , in a least squares sense [8]. The result returned by the Matlab function was a row vector of length  $n+1$  containing the polynomial coefficients in descending powers. Another Matlab function “Polyval” was also used for polynomial evaluation. This function “polyval (p,x)” returned the value of a polynomial of degree  $n$  evaluated at  $x$ . In either case, polyval evaluated  $p$  at each element of  $x$  [8]. The generated curve of modeled fracture toughness post-cured conventionally is shown in Figure 3.

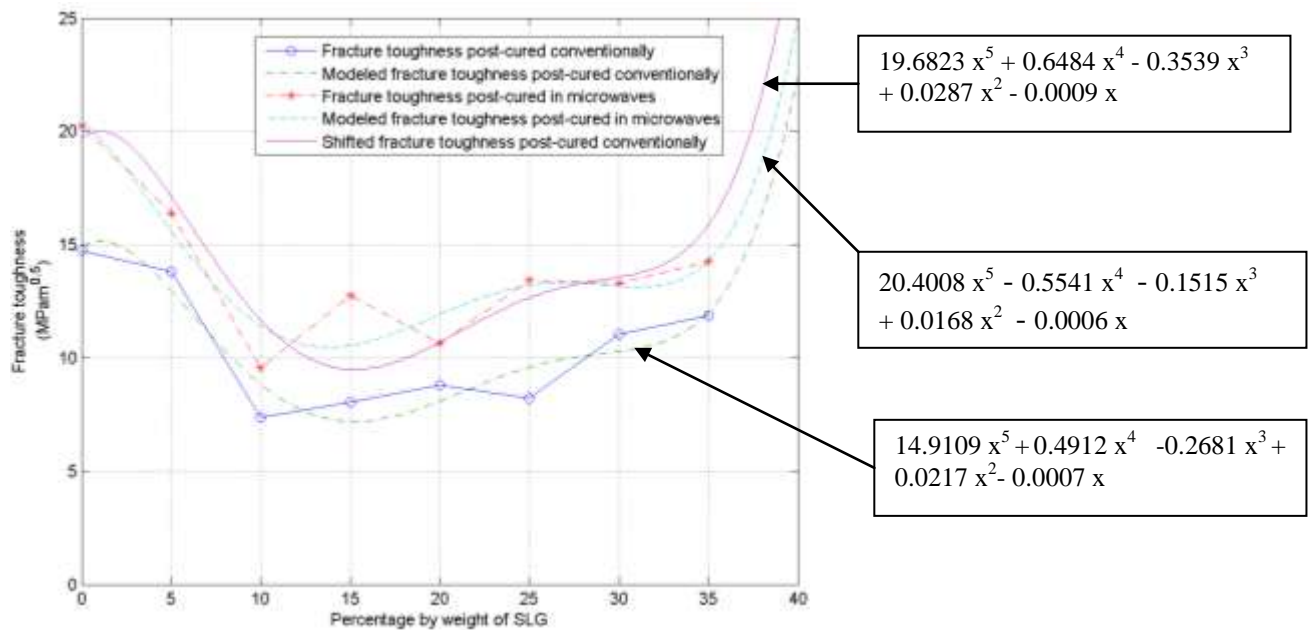
## Results and Discussion

Figure 2 shows the of fracture toughness J2027 (Brendon Chemical) specimens filled with varying weight percentages of E-spheres SLG. Figure 3 shows the mathematical equations (curves) of the fracture toughness of the composites post-cured in microwaves ( $20.4008 x^5 - 0.5541 x^4 - 0.1515 x^3 + 0.0168 x^2 - 0.0006 x$ ) and conventionally ( $14.9109 x^5 + 0.4912 x^4 - 0.2681 x^3 + 0.0217 x^2 - 0.0007 x$ ) respectively. This time order 5 equations were used because order 4 equation could not represent the fracture toughness of the composites post-cured in microwaves accurately. By multiplying the fracture toughness of conventionally post-cured mathematical model (curve) by a constant, a new shifted mathematical model which can approximately represent the fracture toughness of microwave post-cured curve can be generated and it is  $19.6823 x^5 + 0.6484 x^4 - 0.3539 x^3 + 0.0287 x^2 - 0.0009 x$ , which is not too far from the curve of fracture toughness post-cured in microwaves,  $20.4008 x^5 - 0.5541 x^4 - 0.1515 x^3 + 0.0168 x^2 - 0.0006 x$  and the constant for shifting was 1.32.

With the current phenolic resin and raw SLG, it is impossible to add SLG by weight to more than 35% into the composite because the mixture will be too viscous and the two constituents of the composites cannot mix homogeneously. Some chemical treatment of the SLG or modification of the resin may make the addition of SLG by weight to more than 35% into the composite possible and tougher composites will be produced. However, by the mathematical modelling, it is possible to predict the fracture toughness of the composites with more than 35% by weight of SLG as depicted in Figure 3. This will enable one to make a decision whether to chemically treat the SLG or modify the resin to make composites with more than 35% by weight of SLG.

## Conclusion

An order 5 equation has been successfully generated by Matlab to represent the fracture



**Figure 3: Mathematical equation of order 5 obtained from Lagrange’s Method using Matlab**

toughness of composites post-cured conventionally. By using a constant, the mathematical model of fracture toughness of the composites post-cured in microwaves can be generated from that post-cured conventionally and a lot of tedious experiments can be avoided to get the values of the fracture toughness of composites post-cured by microwave irradiation. However, it can be argued that the constant may not be valid if the filler of the composites is changed from SLG to other materials and further study will be done to validate this.

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