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Fracture toughness of polymeric particle nanocomposites: Evaluation of models performance using Bayesian method

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ABSTRACT

This study presents a methodology to evaluate the performance of different models used in predicting the fracture toughness of polymeric particles nanocomposites. Three analytical models are considered: the model of Huang and Kinloch, the model of Williams, and the model of Quaresimin et al. The purpose behind this study is not to recommend which of the three models to be adopted, but to evaluate their performance with respect to experimental data. The Bayesian method is exploited for this purpose based on different reference measurements gained from the literature. The models' performance is compared and evaluated comprehensively accounting for the parameter and model uncertainties. Based on the approximated optimal parameter sets, the coefficients of variation of the model predictions to the measurements are compared for the three models. Finally, the model selection probability is obtained with respect to the different reference data.

1. Introduction

Polymeric nanocomposites (PNCs) are commonly formed by an epoxy matrix reinforced with a nanosized filler. Due to its inherent characteristic of high crosslink density, an epoxy polymer is known to be a relatively brittle material [1]. Nanofillers have shown great improvements in the physical and mechanical properties of epoxy-reinforced PNCs. Specifically, they have increased the fracture toughness compared to pristine epoxy. PNCs have numerous applications in nanotechnology such as: nano-biotechnology, nano-systems, nanoelectronics, and nano-structured materials. Generally, there are three categories of fillers: nanoparticles, nanoplatelet (layered), and nanofibrous materials. For this scale, the surface area - to - volume ratio is significantly large. Therefore, the composite properties are highly modified due to the extreme interfacial area between the nanofiller and the matrix [2]. Several experiments have been carried out in order to study the fracture behavior of polymer/particle nanocomposites ([3–12] among others). On the other hand, researchers developed numerical and analytical methods to get a better understanding of nanocomposite material behavior. A close form formula of energy dissipation due to the interfacial debonding between the particles and matrix was given by Chen et al. [13] considering the effect of particle sizes. Although, the increased fracture energy of rubber-toughened epoxy polymers was calculated by Huang and Kinloch [14], the model has been modified for PNCs by Refs. [7,8,10]. The improvement in the fracture toughness was attributed to two major mechanisms: localized plastic shear banding and debonding of silica nanoparticles. Further experimental studies also have implied this supposition [15–17]. According to the assumption of Williams [18], the energy dissipation is induced by the growth of plastic voids around debonded particles. The author concluded a large toughness increase for nanosize particles. Later, his work has been extended to cylindrical rods and fibres [19,20]. Quaresimin et al. [21] proposed a multiscale approach to predict the overall increase in the fracture toughness taking into account three different damage mechanisms: particle debonding, plastic yielding of nanovoids, and shear banding of the polymer. Based on experimental data gathered from the literature,

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a stochastic approach has been presented to predict the fracture energy of PNCs by Ref. [22].

In general, all models inherently underlie an amount of uncertainties which can be related to the model itself and/or its input parameters. The former might be caused by the simplifications of the physical behavior, while the latter can be related to the number and the stochastic variance of the input parameters. Better predictions and the subsequent decrease in the model uncertainty are expected by introducing more factors in the model (increasing the model complexity). However, the parameters uncertainties become more dominant in this case. In light of this, the model with minimum total uncertainty is the most appropriate model, see Fig. 1 [23].

In recent years, Bayesian method has been introduced as an effective tool for evaluating models considering the model and parameters uncertainties based on measurements as reference data [24–27].

This paper is the first attempt to consider the model and parameters uncertainties in the assessment of the models used for the prediction of the fracture energy of PNCs. It aims at presenting a methodology to evaluate three different analytical models by using the Bayesian method. In particular, Huang and Kinloch model [14], Williams model [18], and the model according Quaresimin et al. [21] are examined. The purpose of the study is not to give a general recommendation which of the three model to use, but to evaluate their performance with respect to experimentally tested data series. The assessment is carried out based on different reference data (experimental measurements) gathered from the literature [3–12]. Nevertheless, the same methodology can be applied to evaluate the three models based on other measurements. The prior probabilities are first estimated considering the uncertainties in the parameters. Then we find the optimum parameter set which results in best fit of models prognoses and in consequence the coefficient of variation of the models predictions to the measurements are estimated. Eventually, the model selection probability is calculated.

The remainder of this paper is organized as follows. In Section 2, the considered models are briefly described. Section 3 presents the method for evaluating the models. Finally, the conclusion of this research is presented in Section 4.

2. Models for predicting the fracture properties of PNCs

Three existing models were chosen to be evaluated; the model of Huang and Kinloch [14], the model of Williams [18], and the model of Quaresimin et al. [21]. Hereafter, they are abbreviated by M_1, M_2, and M_3, respectively. These models have been selected due to their popularity and their applicability to different experimental studies. Moreover, they produce explicit predictions of the enhanced fracture energy of PNCs. Regarding the different theory and mechanism assumed, each of them has its own input parameters in addition to the joint parameters. Table 1 includes the definitions of the parameters and their stochastic variation. The uniform distribution was assumed for the parameters uncertainty. The upper and the lower limits of distributions were mostly proposed according to our previous studies [22,28].

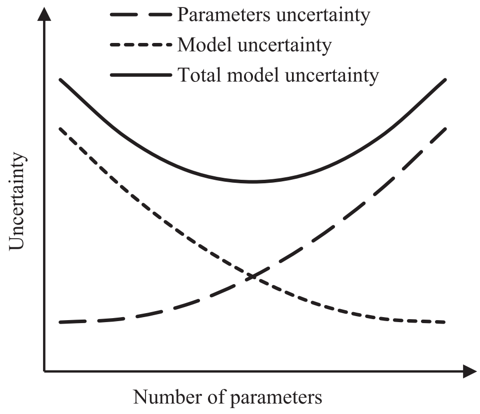

Fig. 1. Variation in model, parameter, and total uncertainties with respect to the number of parameters according to [23].

2.1. Huang and Kinloch

The model according to Huang and Kinloch [14] was first developed for the toughening mechanisms of rubber-modified epoxy polymers and more recently it has been modified for PNCs [7,8,10]. The localized plastic shear banding and debonding of nanoparticles which enable plastic void growth of the epoxy matrix are the two terms that taking part in the overall enhancement in the fracture toughness of PNCs, while rubber-bridging mechanism was disregarded. These two mechanisms are demonstrated in Fig. 2.

The improved fracture energy of PNCs, G_{Ic}, is expressed as

$$G_{Ic} = G_{Im} + \Delta G_s + \Delta G_v \tag{1}$$

where G_{Im} is the fracture energy of the matrix, and ΔG_s and ΔG_v are the contribution from the localized shear banding and the plastic void growth, respectively.

The term ΔG_s is given by

$$\Delta G_s = \frac{1}{2} V_f \sigma_{yc} \gamma_f F'(r_y) \tag{2}$$

where V_f is the volume fraction of the nano-filler, γ_{fm} is the matrix shear fracture strain, and σ_{yc} is the yield stress of the epoxy matrix under compression, which related to the tensile yield stress, σ_{ym}, by Ref. [5].

$$\sigma_{yc} = \sigma_{ym}\left(\frac{\sqrt{3}+\mu_m}{\sqrt{3}-\mu_m}\right) \tag{3}$$

μ_m is a material constant (pressure coefficient).

The parameter $F(r_y)$ is a geometric term given by Ref. [15].

$$F'(r_y) = r_y\left[\left(\frac{4\pi}{3V_f}\right)^{1/3}\left(1-\frac{r_n}{r_y}\right)^3 - \frac{8}{5}\left(1-\frac{r_n}{r_y}\right)\left(\frac{r_n}{r_y}\right)^{5/2} - \frac{16}{35}\left(\frac{r_n}{r_y}\right)^{7/2} - 2\left(1-\frac{r_n}{r_y}\right)^2 + \frac{16}{35}\right] \tag{4}$$

where r_n (=d_n/2) is the radius of nanoparticles and r_y is the radius of the plastic zone at the crack tip at fracture in the PNCs

$$r_y = \left(1+\frac{\mu_m}{\sqrt{3}}\right)^2 r_{ym} K_{vm}^2 \tag{5}$$

In Eq. (5), r_{ym} is radius of the plastic zone of the unmodified epoxy matrix estimated by Irwin's model [29] and K_{vm} is the maximum stress concentration factor of the von Mises stress in the matrix.

The term ΔG_v is calculated by