STATISTICAL MODELING OF TENSILE PROPERTIES OF TALC-FILLED POLYPROPYLENE BASED ON MULTIVARIATE REGRESSION AND NEURAL NETWORK ANALYSES

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Abstract

In this paper, tensile properties of homo polypropylene (PP) with respect to talc filler content were predicted using regression model and neural network model. Talc content, tensile speed, Differential Scanning Calorimeter (DSC), Gel Permeation Chromatography (GPC) and rheometer data were used as modeling input factors. 2 different multiple regression models and 1 neural network model were established and the models were compared quantitatively by average error rate (AER). The results showed high reliability for all models but neural network models were determined as the most meaningful model.

Introduction

Recently, polymeric materials are widely used in many industrial fields. Unlike metal, data of polymers concerning material property are insufficient. Especially, polymers have many differences in material properties with metals. Therefore, traditional approaches are restricted and constructing databases of polymers is becoming an important issue.

Polymer materials have different structures and properties according to its monomer or additive. Melt properties are determined by the intrinsic properties of the material. For these reasons, researches have been focused on evaluating intrinsic properties of materials [1]. For example, melt flow index (MFI), number average molecular weight (Mn) and weight average molecular weight (Mw) can be used. Since the properties of polymers are attributed to its structure, it is very important to select proper parameters to estimate the material properties well. Crystallinity is one of the important factors related to material properties. For semi-crystalline polymers, characteristics of crystalline phase such as crystallinity and size of spherulite should be considered [2-5]. Material properties are also affected by structural factors which is highly dependent on manufacturing process.

In this study, design of experiment (DOE) was used to determine MI and talc content of PP composite. Correlations of the material properties of composite with analysis parameters were statistically evaluated by regression models and neural network models.

Materials and Experiments

Specimens were prepared using homo PP with various talc content. DOE and result analysis were conducted by JMP software. To minimize the number of experiment and obtain 2nd order model, 7 different specimens with 3-level factor were prepared. Upper and lower limit were set and response surface design of 2 factors of 3 level were used. Designed test conditions (MI : 5, 27.5, 50 g/10 min, talc content : 0, 25, 50 %) are illustrated in Figure 1.

Tensile tests were conducted according to ISO 527 with gauge length 75 mm, thickness 4 mm and width 10 mm. Crosshead speeds were 5, 50, 500 mm/min. MTS 810 servo-hydraulic test machine was used and tests were repeated for 5 times each. Elastic modulus and yield stress were measured from the test. Figure 2 is a schematic of tensile specimen and Table 1 shows design table and test conditions.
Crystallinity was measured by TA Q20. In nitrogen atmosphere, samples were heated from 30 °C to 200 °C and kept for 5 minutes. After isothermal process, samples were cooled to 30 °C and reheated to 200 °C. Between cooling and 2nd heating cycle, the temperature was fixed to 30 °C for 5 minutes. Heating and cooling rate were 10 °C/min. To measure molecular weight and rheology properties, HT-GPC agilent PL-220 rheometer TA ARES-G2 were used. Frequency sweep type rheology test was conducted in 210 °C. Zero shear viscosity, K and m were obtained from equation (1). M_n, M_w, M_z and polydispersity (PD) were obtained from GPC [6].

\[
\eta = \eta_\infty + \frac{\eta_0 - \eta_\infty}{1 + (K \gamma)^m}
\]  

(1)

Results and Discussion

Regression Model

Statistical models for mechanical properties were established by material analysis parameters. 7 different specimens were tested in random order. Regression model and neural network model were obtained from JMP software. Regression models were established by response surface analysis method. Tensile speed, MI, talc content, DSC, GPC and rheology parameters were used as input factors. Screening analysis was conducted to find major factors of tensile properties. 2nd order polynomial regression model was optimized by eliminating the factors that are statistically less relevant.

Figure 3 and Figure 4 show the actual test results and predicted values of polynomial regression model. It can be found that the models predict the results well. Figure 3 shows two models for elastic modulus. Tensile speed-MI-talc content and tensile speed-M_w-crystallinity were used respectively. Figure 4 is the results of tensile strength. Standard deviation increased in modulus models but still shows meaningful results.
Neural Network Model

In neural network model, 2/3 of the data obtained from the test are used for training the model and the rest are used for validation. Data are randomly selected to construct model. The process was repeated for several times and the model with the least $R^2$ value difference between training and validation was selected. Models are composed of input layer, hidden layer with 3 nodes and output layer (Figure 5). The input nodes of a neural network model include test speed, talc content, DSC, GPC and rheometer data. Output nodes are tensile modulus and strength.

Figure 6 and Figure 7 show the results obtained from neural network models. It can be found that the results show more linearity than regression models.
Figure 7. Predicted tensile stress of Neural networks model.

Comparison of Prediction Models

Quantitative evaluation of prediction quality of regression models is conducted by various means such as F-test by analysis of variance (ANOVA), coefficient of determination, correlation coefficient, and average error rate (AER) [7]. In this research, AERs of each model were evaluated and compared. AER can be calculated as [8]:

\[
AER(%) = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{y_i - \hat{y}_i}{y_i} \right| \times 100
\]  

(2)

where \( n \) = total number of tests, \( y \) = measured value and \( \hat{y} \) = predicted value. The less the AER, the better the model.

Table 2 shows AERs of 2 regression models and 1 neural network model. In regression model, modulus is predicted by tensile speed-MI-talc content with error of 3.95 %. Tensile stress can be estimated by tensile speed-talc content-Mw with 1.59 % error. Neural network model predicted the properties with less error (2.73 %, 1.27 % respectively). It can be concluded that the neural network model has advantages over regression model in non-linear properties [9].

<table>
<thead>
<tr>
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<th>Regression Model</th>
<th>Neural Network Model</th>
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<tbody>
<tr>
<td></td>
<td>(a)</td>
<td>(b)</td>
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<tr>
<td>Modulus</td>
<td>3.95%</td>
<td>4.93%</td>
</tr>
<tr>
<td>Tensile stress</td>
<td>1.59%</td>
<td>1.75%</td>
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</table>

Conclusions

Tensile modulus and yield stress of PP with respect to talc content were predicted. Modeling input factors were talc content, tensile speed, DSC (crystallinity, heat of fusion), GPC (Mn, Mw, Mz, PD) and rheometer (zero shear viscosity, K, m). Multiple regression model and neural network model were used. Screening analysis was conducted to find major factors in tensile properties. 2 different multiple regression models and 1 neural network model were constructed. Models were compared quantitatively by AER. Neural network model showed less AER than multi regression models because of non-linearity (2.73 % for tensile modulus and 1.27 % for yield stress).

References