Yield Strength Prediction for Thermoplastic Composites based on a Sparse Fuzzy Model

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Abstract-Nowadays thermoplastic composites are commonly used owing to their good mechanical properties, which can be ensured only by the proper mixing of different types of materials. In this paper, we present the results of our studies regarding the fuzzy modeling of the relation between the yield strength and the amount of the used components (ABS, polycarbonate, multiwall carbon nanotube). The initial rule base was created using FCM clustering and the parameters were tuned by RBE-SI that applies a hill-climbing approach and enriches the rule base with new rules if it is necessary. Owing to the possible sparse character of the rule base the fuzzy rule interpolation based FRIPOC method was used as inference technique. The model was validated by applying it to an independent set of test data.

Keywords-yield strength, fuzzy modeling, FRIPOC, RBE-SI

I. INTRODUCTION

Nowadays polymers are very important materials; they are used for different purposes. The variety of plastics is enormous. In some cases it is difficult to achieve the requirements of the costumers. Sometimes it is important to prepare composites by mixing different types of materials.

The carbon nanotube is a very interesting and important material. It has significant mechanical properties. Several researchers work with single wall and multiwall carbon nanotubes. In the last ten years polymer – carbon nanotube blends were prepared and investigated [18][22][29]. These composites are often used to increase the polymer's conductivity [1][5][27] and decrease its resistance, electrostatic discharge can be avoided. It was also discovered that the mechanical properties (modulus, strength) can be enhanced by adding carbon nanotube to virgin polymer [5][8]. In addition, among other properties the thermal stability and fire resistance can be influenced favorably as well by using carbon nanotube [16][23][36].

The prediction of mechanical properties is of great importance in composite production. Soft computing techniques like fuzzy rule based systems (FRBS), artificial neural networks (ANN) and evolutionary algorithms (EA) have been applied successfully for modeling of different non-linear phenomena where one does not know the exact mathematical formula that describes the relation between the input and output variables of the model, but there exist human expertise or experimental data are available.

The advantages of FRBSs can be summarized in the following points.

- They can incorporate human knowledge as well as knowledge induced from numerical data obtained by the observation of the original phenomena.
- The model is described by fuzzy rules that are easyly interpretable and analyzable.
- Each fuzzy rule represents a local model, which results in robustness and good approximation capability; the modification of a single parameter does not alter the whole model.

There is a broad literature reporting successful practical applications of FRBSs. For example Kovács and Kóczy [21] developed a fuzzy rule interpolation (FRI) based model for behavior-based control structures; Johanyák, Parthiban, and Sekaran [15] constructed fuzzy models for an anaerobic tapered fluidized bed reactor; Hládek, Vaščák and Sinčák [9] proposed a hierarchical multi agent control system based on rule based fuzzy system for pursuit-evasion task; etc.

This paper presents the results of our research aiming the generation of a fuzzy model in order to support the prediction of thermoplastic composites' yield strength as a function of the percent amount of the components. The model applies the percentage of the nanotube and ABS as input parameters. The amount of the third component (polycarbonate) is a dependent variable; therefore it was not used during the calculations.

The rest of this paper is organized as follows. Section II. presents the experiments. Section III. introduces the methods and techniques used in course of the design and identification of the fuzzy model. The results are discussed in section IV.

II. EXPERIMENTS

In the experiments polymer nanocomposites were prepared. ABS (POLYMAN HH 3, Polyman Plastics Inc.), polycarbonate (PC, ANJALON J100V, J&A Plastics GmbH) were used as matrix materials. Multiwall carbon nanotube master batch (MB-6015-00, Hyperion Catalyst, USA) was used to prepare the composites. Concentration series with 0%, 1%, 1.5% carbon nanotube content were prepared to investigate the effect of the components.

The mixing of polymers was carried out in melt to achieve homogeneous properties. We used a special mixing unit called Infinitely Variable Dynamic Shear Mixer (IDMX) [31] to produce blends. The mixing instrument consists of the dynamic unit and a satellite extruder. The extruder is a Collin Teach-Line E20T. The single screw extruder pumps the melt into the dynamic mixer. The mixer has its own drive and a screw feed section which takes the melt streams and conveys them into the mixer elements consisting of rotors and stators. The setup of the mixing elements generates high shear to give dispersive and distributive mixing of the components. The test pieces were injection molded by ARBURG Allrounder 270 U 350-70. The melt temperature was 260 °C, the mould temperature was 40° C.



Figure 1 SEM micrograph of the fractured surface of the composite containing 1% nanotube, 90% ABS, and 9% PC

The structure and mechanical properties of the materials were investigated. In order to study the structural properties of the test pieces we broke them under liquid nitrogen. We prepared scanning electron microscopic (SEM) pictures to investigate the fractured surface of the composites. A field-emission SEM (FESEM, Hitachi-S4700) was applied for this task.



Figure 2 SEM micrograph of the fractured surface of the composite containing 1% nanotube, 10% ABS, and 89% PC

The yield strength (YS) of the composites was measured by INSTRON 4482 equipment. SEM micrographs of the fractured sample composites containing carbon nanotube are shown in Fig. 1 and Fig. 2. The sample preparation was carried out in the same way as in [3]. The carbon nanotube can be seen on the fractured surfaces. We did not find any sign of agglomerates in the materials.

III. FUZZY MODELING

A. Fuzzy inference

In course of fuzzy modeling one can choose from a wide variety of inference methods. They can be divided into two main groups depending on their ability to cope with sparse rule bases. A fuzzy rule base is sparse (e.g. Fig. 3) when for some observations there is no rule that could be applied, i.e. there is no rule whose antecedent part would at least intersect the observation.



Figure 3 Sparse rule base

The members of the first group are the so called classical compositional methods like Zadeh's [35] or Mamdani's [24] inference techniques. They require a full coverage of the input space by the known rules.

The members of the second group can use a more compact representation of the knowledge incorporated in the rule base and so they are capable to reason in sparse rule bases as well. This feature presents a large application potential in fuzzy control [26] as well. These methods determine the conclusion using approximation based reasoning, usually a kind of fuzzy rule interpolation (FRI) taking into consideration two or more rules situated in closer or wider neighborhood of the observation. Frequently used FRI methods are the KH method [17]; the vague environment based FIVE developed by Kovács [20]; the Generalized Methodology of fuzzy rule interpolation (GM) developed by Baranyi, Kóczy and Gedeon [2]; the transformation based technique published by Chen and Ko [6]; the polar cut based FRIPOC suggested by Johanyák and Kovács in [11]; the IGRV developed by Huang and Shen [10]; the LESFRI published by Johanyák and Kovács in [12]; the interpolation method (developed by Kovács [19]) that extended the fuzzy interpolation to the general metric spaces; as well as the IMUL method suggested by Wong, Tikk, Gedeon and Kóczy [34].

B. FRIPOC

We used the Fuzzy Rule Interpolation based on POlar Cuts (FRIPOC) [11] method in course of the fuzzy model identification. Its main idea is that it determines the shape of the conclusion by its polar cuts. The method follows the concepts of the generalized methodology of fuzzy rule interpolation (GM) developed by Baranyi, Kóczy and Gedeon [2]. It identifies the position of the fuzzy sets by their reference points using the centre of the core as reference point. The conclusion is determined in two steps.

Firstly, one interpolates a new rule whose antecedent sets are in the same position as the current input sets (observation) in each antecedent dimension. The antecedent and consequent sets of the new rule are determined by set interpolation using the technique FEAT-p. The positions of the consequent sets are calculated by an adapted version of the Shepard interpolation [30]. Secondly, one calculates the shape of the conclusion in the second step by the SURE-p method using the observation and the interpolated rule.



Figure 4 Reference point and polar cut

1) Polar cut

The methods FEAT-p and SURE-p use polar cuts in course of the calculation of the shape of the fuzzy sets. The concept of polar cuts is based on the application of a polar coordinate system that is placed at the reference point of the set (Fig. 4). A polar cut describes one point on the shape of a fuzzy set. It consist of a value pair $\{\rho, \theta\}$, where ρ is the polar distance of the point and θ is the corresponding polar angle. Similar to the case of α -cuts an extension and resolution principle can be formulated for polar cuts as well stating that each convex fuzzy set can be decomposed into polar cuts and can be composed from polar cuts.

2) The FEAT-p method

The Fuzzy sEt interpolATion based on polar cuts aims the creation of a new fuzzy set in a given point of a universe of discourse called interpolation point. The calculations are based on a supposed regularity between the known sets of the partition. It also uses the concept of Linguistic Term Shifting (LTS) and polar cuts.

Conform to LTS first all known sets of the partition are shifted horizontally in order to reach the coincidence between their reference points and the interpolation point. Next the shape of the new set is calculated by its polar cuts. Each polar length is determined as a weighted average of the corresponding polar lengths of the overlapping known sets. The weighting is based on the original distance of the sets from the interpolation point.

3) The SURE-p method

Generally the antecedent sets of the interpolated rule are not identical with the observation sets. Therefore the conclusion is determined by a special single rule reasoning method that modifies the consequent sets of the new rule taking into consideration the similarity between the observation and the rule antecedent sets.

The Single rUle REasoning based on polar cuts first calculates for each polar cut and for each input dimension the difference between the polar length of the observation and the polar length of the rule antecedent set. Next an average difference is determined for each polar level and the consequent polar lengths are modified by this resulting difference. The final shape of the conclusion fuzzy set is determined by a control and correction algorithm that ensures the avoidance of the abnormal set shapes.

C. Fuzzy rule base generation from sample data

In course of fuzzy model identification one determines the structure of the rule base, the number of rules as well as the membership function types and parameters of the fuzzy sets referenced in the rules. In course of the rule base generation one can apply one of the following two approaches. The first one divides the task into two separate steps, i.e. the structure definition and the parameter identification (e.g. Precup, Doboli and Preitl [25]; or Botzheim, Hámori and Kóczy [4], or Škrjanc, Blažič and Agamennoni [28]).

The second approach works incrementally by simultaneously modifying the structure and the parameters, i.e. introducing or eventually eliminating rules and tuning the parameters of the membership functions (e.g. Johanyák and Kovács [13]).

In course of the development of the fuzzy model we used a hybrid approach adopted from two previously published methods, i.e. ACP [14] and RBE-SI [13]. Further on we will review those parts of them that were applied in our case. The key idea was to create first a starting rule base using a clustering based technique and next to try finding the quasi-optimal parameters of the rules, which step also could involve creation of new rules.

1) Creation of the initial rule base using fuzzy clustering

In course of the initial rule base generation the approach proposed in [7] and in [33] was followed. Firstly, a onedimensional FCM clustering was done in the output dimension followed by the identification of the consequent linguistic terms, and the rules. The main steps of the algorithm are presented in Fig. 5.

- Determination of the optimal cluster number in the output dimension
- FCM clustering of the output data
- Identification of the output partition's fuzzy sets
- For each consequent linguistic term projection into the antecedent space
 - o Data subset identification
 - o In each antecedent dimension
 - Determination of the optimal cluster number
 - FCM clustering
 - Rule creation
- In each antecedent dimension
 - Examination of the cluster center mergeability
 - o Identification of the antecedent fuzzy sets

Figure 5 Algorithm for the initial rule base generation

2) Determination of the optimal cluster number

The FCM clustering requires as input parameter the number of the clusters to be identified. In most of the cases this a priori knowledge is not available. Therefore usually cluster validity indices are applied for the determination of the quasi-optimal cluster number. A comprehensive study of the potential indices was made by Wang and Zhang in [32] for the FCM clustering. ACP (Automatic fuzzy system generation based on fuzzy clustering and Projection) [14] uses an enhanced version of the index proposed by Chong, Gedeon and Kóczy [7]. One estimates the starting cluster number by the *FS* index

$$FS = \sum_{j=1}^{c} \sum_{k=1}^{M} (u_{jk})^{m} \cdot ((x_{k} - v_{j})^{2} - (v_{j} - \overline{v})^{2}), 2 \le c \le M$$

where *M* is the number of the sample data rows, *c* is the cluster number, *m* is the fuzzy exponent, v_i is the center of the *i*th cluster, u_{jk} is the membership value of the *k*th point in the *j*th cluster and

$$\overline{v} = \frac{\sum_{j=1}^{c} v_j}{c}.$$

One has to calculate the *FS* index for a wide range of cluster numbers. That cluster number is chosen for which *FS* takes its minimum. Next, for each neighbouring cluster centre pair one examines their mergeability using the cluster merging index

$$P(v_m) = \sum_{j=1}^{M} e^{-\left(\frac{v_m - x_j}{r_i}\right)}$$

Supposing that v_m would be the centre of the to be merged clusters having the centres v_i and v_k , the two clusters can be merged when $P(v_m) < P(v_i)$ and $P(v_m) < P(v_k)$.

3) Identification of a partition's fuzzy sets

In this step our aim is to create a Ruspini type partition using trapezoidal shaped membership functions in each dimension. After FCM one calculates the α -cuts of the clusters at the level of α =0.85. The lower and upper endpoints define the core of a set taking also into consideration the lower and upper bounds of the actual dimension



In order to ensure the Ruspini character of the partition the endpoints of the support are defined to be identical with the core endpoints of the neighbouring linguistic terms

$$\inf \left\{ \begin{bmatrix} A_j \end{bmatrix}_0 \right\} = \begin{cases} x_{\min} & \text{if } j = 1\\ \sup \left\{ \begin{bmatrix} A_{j-1} \end{bmatrix}_1 \right\} & \text{if } j = 2,...,c ,\\ \sup \left\{ \begin{bmatrix} A_j \end{bmatrix}_0 \right\} = \begin{cases} x_{\max} & \text{if } j = c\\ \inf \left\{ \begin{bmatrix} A_{j+1} \end{bmatrix}_1 \right\} & \text{if } j = 1,...,c-1 . \end{cases}$$

Fig. 6 illustrates the process.

4) Projection into the antecedent space

The rules are created based on the projection concept. In this subsection we describe the necessary steps. Having the consequent linguistic terms already determined the next step is done on a one-by-one basis for each of them. Firstly, one selects all of the data rows whose output falls into the support of the current set. Next, in case of each antecedent dimension one does a one dimensional FCM clustering. Each cluster is labelled with an identifier of form $A_{i,j,k}$, where *i* is the number of the antecedent dimension, *j* is the number of the consequent set and *k* is the number of the current cluster within its group. Thus one can create two or more rules in case of each consequent linguistic term, whose form is

$$R_m : IF \ a_1 = A_{1,j,k_1} \ AND \dots AND \ a_N = A_{N,j,k_N}$$
$$THEN \ b = B_j$$

After the initial rule creation one sorts in ascending order the recognized cluster centres, which is followed by a relabeling in each antecedent dimension. The new labels are of form A_{ij} , where *i* is the number of input dimension and *j* is the number of the cluster in its dimension. The final sets are determined by the method presented in the previous subsection.

5) Parameter tuning

Having an initial rule base we used the tuning algorithm of RBE-SI (Rule Base Extension based on Set Interpolation) [13]. The method applies a hill-climbing type approach for the identification of the quasi-optimal parameters. Besides, if the amelioration of the performance index between two iteration cycles becomes too small and the step size is also too small a new rule is generated. Fig. 7 presents the applied algorithm.

The algorithm stops in two cases, either when the performance of the fuzzy system becomes better than a threshold value ($PI_{prescribed}$) or when the number of the iteration cycles exceeds its maximum allowed value (*IterMax*). The new value of the current parameter is calculated either by decreasing or by increasing the original value by a predefined step. Its original value depends on the range of the current partition (DR_i)

$$st_i = C \cdot DR_i, \ C \in [C_{\min}, 1]$$
$$C_{\min} = \frac{10^{-dn}}{\min_{i \in [1, N+1]} (DR_i)},$$

where *C* is a parameter of the method, *dn* is the number of applicable decimals in case of the given dimension.



Evaluate original fuzzy system ($PI_{best} = PI_0$)

For each antecedent and consequent dimension

6) Performance evaluation

IterNo=1

.

Define step size

START ITERATION

There are several choices for the performance evaluation of a fuzzy system. Their common feature is that they create a single number that expresses how far the sample output points from the calculated output points are. The most common choice is the root mean square of the error

$$PI_{RMSE} = \sqrt{\frac{\sum_{j=1}^{M} (y_j - \hat{y}_j)^2}{M}},$$

where *M* is the number of the sample data points, y_j are the sample output values, and \hat{y}_j are the calculated output points.

7) New rule creation

The RBE concept extends the rule base in course of an iterative process. A new rule will describe that point of the consequent space where the deviation is the biggest between the sample data and the output calculated by the fuzzy system. RBE-SI uses set interpolation for the determination of the shape of the new rule's sets. The applied set interpolation type is strongly related to the applied inference type. Thus for example in case of FRIPOC [11] one uses FEAT-P or in case of LESFRI [12] FEAT-LS is applied.

IV. RESULTS AND DISCUSSION

The purpose of our research was to create a sparse fuzzy model aiming the prediction of the yield strength (YS) in function of the percent amount of the components in thermoplastic composite production. Although the mixture contained three components, namely the multiwall carbon nanotube, the ABS, and the polycarbonate (PC) the model uses only two of them (nanotube and ABS) as input variable because the percent amount of the PC is a dependent variable.

We divided the experimental results into two separate data sets, one for fuzzy system identification (training) and one for system validation (testing) purposes. The training data set contained the results of 31 experimental setups. The experiments were carried out with 10 replications, which results in total 310 experiments. The testing data set contained the results of 9 experimental setups. In its case the experiments were carried out also with 10 replications, which resulted 90 experiments.







Figure 9 Calculated and measured yield strength values in case of the training data and the final fuzzy system

In order to avoid the overfitting of the model to the training data set we monitored not only the performance of the different fuzzy systems in case of the training data set but we also followed their goodness in case of the testing data set (see Fig. 8). We chose that parameter values for which the best results were shown in case of the test data. The performance of the system is characterized in Table I. Fig. 9 shows the calculated and sample yield strength values in case of the training data.

TABLE I. PERFORMANCE OF THE FUZZY MODEL

	Training	Testing
RMSE	0.4854	1.5895

V. CONCLUSIONS

The paper presented the application of RBE-DSS rule base identification and FRIPOC fuzzy rule inference methods for fuzzy modeling of the relation between the yield strength of the thermoplastic composites and the percent amount of their components. The models were evaluated using RMSE as performance indicator. Conform the testing results the generated model proved to be good predictor of the studied process.

ACKNOWLEDGMENT

This research was partly supported by the National Office for Research and Technology (Gábor Baross programme), the National Scientific Research Fund Grant OTKA 77809 and the Normative Application of R&D by Kecskemét College, GAMF Faculty.

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