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Mechanical Properties Prediction of Thermoplastic Composites using Fuzzy Models

Z.C. Johanyák*, A.M. Ádámné**

[*] Institute of Information Technologies, Kecskemét College, Faculty of Mechanical Engineering and Automation, Izsáki út 10., H-6000 Kecskemét, Hungary
Phone: (+3676) 516-413, Fax: (+3676) 516-399, E-Mail: johanyak.csaba@gamf.kefo.hu, WWW: http://johanyak.hu

[**] Institute of Metal and Polymer Technology, Kecskemét College, Faculty of Mechanical Engineering and Automation, Izsáki út 10., H-6000 Kecskemét, Hungary
Phone: (+3676) 516-392, Fax: (+3676) 516-399, E-Mail: major.andrea@gamf.kefo.hu, WWW: http://www.gamf.hu/portal/?q=gamf/oktato/adamne_major_andrea

***Abstract* – The ability to predict mechanical properties of thermoplastic composites in order to satisfy the performance requirements is of great importance in course of the design. In this paper, a general method group for data driven fuzzy modeling and its application is presented. Two low complexity fuzzy models were generated for the prediction of Charpy impact strength and yield strength as a function of the percent amount of the components. The models take as input parameters the percentage of the nanotube and ABS**

***Keywords:* thermoplastic composite, fuzzy modeling, LESFRI, RBE-DSS,**

I. INTRODUCTION

In the 19. century polymers were used as synthetic substitute materials instead of raw materials. Nowadays polymers are very important materials; they are used for different purposes. The variety of plastics is enormous; however, in some cases there is no pure material to fulfill all the requirements. In these cases it is important to prepare the desired material by mixing pure polymeric materials with fullerenes in order to reach the desired mechanical properties.

One type of fullerenes, the carbon nanotube is in the focus of the researchers of polymer blends in the last ten years [1][2]. Carbon nanotube-polymer composites are often used owing to the increase of the polymer's conductivity [3][4][5] and decrease of its resistance. Thus electrostatic discharge can be avoided. It was also discovered that the mechanical properties (modulus, strength, etc.) can be enhanced by adding carbon nanotube to virgin polymer [6][7]. In addition, among other properties the thermal stability and fire resistance can be influenced favorably as well by using carbon nanotube [8][9][10].

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 genetic programming (GP) 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 exists human expertise or experimental data is available.

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

1) They can incorporate human knowledge as well as knowledge induced from numerical data obtained by the observation of the original phenomena.

2) The model is described by fuzzy rules that are easy interpretable and analyzable by humans.

3) Each fuzzy rule represents a local model, which results in robustness and good approximation capability because the modification of a single parameter does not alter the whole model.

4) A suitable initial parameter set determined by human experts can substantially speed up the training process.

There is a broad literature reporting successful practical applications of FRBSs. Kovács and Kóczy [13] developed a fuzzy rule interpolation (FRI) based model for behaviour-based control structures. Johanyák, Parthiban, and Sekaran [14] constructed fuzzy models for an anaerobic tapered fluidized bed reactor. Wong and Gedeon [15] as well as Johanyák and Kovács [16] developed FRBSs for prediction of petrophisycal properties. Blažič and I. Škrjanc [35] developed a fuzzy model based predictive control algorithm applicable for processes with strong nonlinear dynamics and high transport delays. Hládek, Vaščák and Sinčák [36] proposed a hierarchical multi agent control system based on rule based fuzzy system for pursuit-evasion task.

In this paper, we present the results of our research aiming the generation of fuzzy models in order to support the prediction of mechanical properties of thermoplastic composites as a function of the percent amount of the components. Two models were generated, one for Charpy impact strength and one for yield strength. Both models apply 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 order to investigate variation of the Charpy impact strength (CIS) and yield strength (YS) of the composites in function of the component's percent amount we created an incomplete full factorial experimental design. The incompleteness derived from the constraint that the sum of the component's percent amount had to be 100%.

The components were POLYMAN HH 3 also known as ABS, the Multiwall Carbon nanotube master batch (MB-6015-00, Hyperion Catalyst, USA) and the polycarbonate (PC). The ABS and PC polymers were used as matrix materials. We defined three levels for the percent amount of the nanotube (0%, 1%, and 1.5%) and eleven levels in case of (0%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, and 100%) ABS. The full factorial experiment plan contained 33 settings from which 30 were executable due to the incompatible levels (see the above mentioned constraints). Each setting was tried ten times. The experiments were carried out in random order. In course of the modeling the average value for each setting was taken into consideration as setting results.

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) [11] 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 260º C. The mould temperature was 40º C.

In order to study the mechanical properties of the test pieces we broke them under liquid nitrogen. The yield strength was determined by an INSTRON 4482 equipment. The Charpy impact strength was determined as well using a swinging pendulum (Charpy pendulum).

We also 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. 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 [12]. The carbon nanotube can be seen on the fractured surfaces. It is important to emphasize that the distribution of the nanotube in the matrix material is more or less uniform. We did not find any sign of agglomerates in the materials.

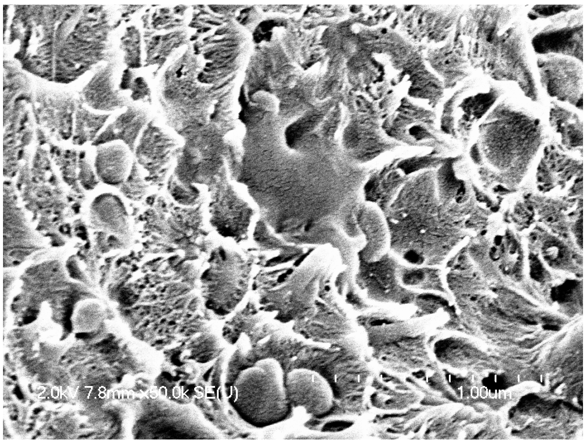

Fig. 1. SEM micrograph of the fractured surface of the composite containing 1% nanotube, 90% ABS, and 9% PC

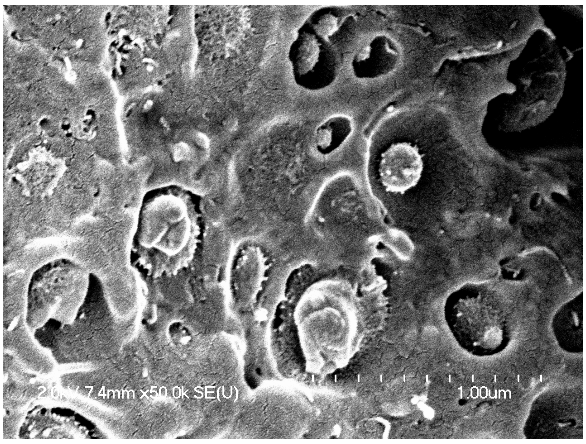

Fig. 2. SEM micrograph of the fractured surface of the composite containing 1% nanotube, 10% ABS, and 89% PC

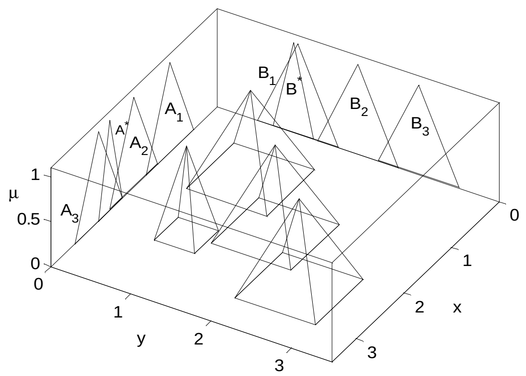

Fig. 3. Sparse fuzzy rule base

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. Fig. 3 illustrates the two dimensional antecedent space of a sparse fuzzy rule base that contains three rules whose antecedents are represented by pyramids. In case of the observation $\{A^*, B^*\}$ none of the rule antecedents intersects the observation.

The members of the first group are the so called classical compositional methods like Zadeh's [17], Mamdani's [18] or Larsen's [19] 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, they are capable to infer in sparse rule bases as well. This feature presents a large application potential in fuzzy control [34] 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. These methods also form two subgroups, the so called one-step and two-step techniques.

The one-step FRI techniques determine the conclusion directly from the observation and the rules taken into consideration. Here belongs e.g. the linear interpolation proposed by Kóczy and Hirota [20], the vague environment based reasoning FIVE developed by Kovács [21], or the IMUL method suggested by Wong, Tikk, Gedeon and Kóczy [22].

The two-step FRI methods follow the concept of Generalized Methodology of fuzzy rule interpolation (GM) developed by Baranyi Kóczy and Gedeon in [23]. In the first step they interpolate a new rule in the position of the observation and next they calculate the conclusion using a special single rule reasoning technique. Typical members of this group are the technique family suggested in [23], LESFRI published by Johanyák and Kovács in [24], IGRV developed by Huang and Shen [25], the transformation based technique published by Chen and Ko [37] as well as the polar cut based FRIPOC suggested by Johanyák and Kovács in [26].

B. LESFRI

We chose LESFRI [24] as inference technique owing to its low computational complexity, its ability to preserve the characteristic shape type of a partition, and good practical experiences gathered in course of previous fuzzy modeling problems.

Conform the concepts of GM LESFRI interpolates first a new rule in the position of the observation. The same position here means that in each antecedent dimension the reference point of the antecedent fuzzy set of the new rule will be identical with the reference point of the observation. The calculations are done independently in each antecedent dimension using the set interpolation technique FEAT-LS. FEAT-LS first shifts virtually all linguistic terms of the partition (see Fig. 4) in order to reach a coincidence between the reference point of the observation and the reference points of the shifted sets. The left and right flanks of the new set are determined separately.

The next step of LESFRI is the compilation of an α-level set that contains all levels corresponding to the break-points of the shifted sets on the current (left or right) side. One calculates a characteristic point of the new set for each α-level so that the distances between the α-cut endpoints of the shifted sets and the new characteristic point to be minimal by the means of the weighted least squares methods. The weighting expresses that the linguistic terms situated originally in farther portions of the partition should have a weaker effect on the result than those situated originally in closer neighborhood of the observation. The rest of the set shape is determined by connecting the neighboring characteristic points with lines. After determining the shape of the antecedent sets of the

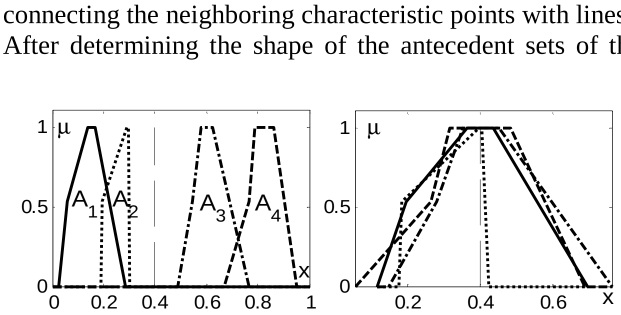

Fig. 4. Linguistic term shifting

new rule one calculates the position (reference) point by the crisp Shepard interpolation [27], which calculates the new point as a weighted average of the reference points of the known rules' consequents. Next the shape of the conclusion is determined using the same set interpolation technique as in the case of the antecedent sets.

In the second step of LESFRI the conclusion is generated by a special revision technique called single rule reasoning based on the method of least squares (SURE-LS). Single rule reasoning can be applied when the reference points of an observation and the reference points of a rule antecedent coincide in all input dimensions. In such circumstances the conclusion is generated by a modification the rule consequent's shape. This modification also called revision should be related to the similarity/dissimilarity of the observation and rule antecedent sets. However, the revision does not alter the reference point of the consequent set.

SURE-LS applies an α-cut based approach for this task. It uses a set of α-levels compiled together by taking into consideration the break-point levels of all antecedent dimensions and the current consequent partition. The calculations are done separately for the left and right flanks. On each side for each level it calculates the weighted average of the distances between the endpoints of the α-cuts of the rule antecedent and the observation set. The weighting makes possible to take into consideration the different antecedent dimensions (input state variables) with different influence.

The basic idea of the method is the conservation of the weighted average differences measured on the antecedent side. These differences are measured in horizontal direction and the revision results in an intermediate set or an array of points. The conclusion with the desired shape type is calculated from these applying the method of Least Squares. In cases when the rule antecedent fits the observation perfectly the conclusion will be identical with the consequent of the rule.

IV. FUZZY MODEL IDENTIFICATION

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. One can find a wide variety of applicable methods in the literature. The selection first depends on the demand whether a full coverage of the input space is required or not, which on its turn lays on the chosen inference technique. In our case we chose LESFRI for fuzzy reasoning and therefore a low complexity sparse rule base containing only the relevant rules is sufficient.
One can produce a sparse fuzzy rule base basically in two ways. The first (e.g. [28]) starts from a completely covering rule base and reduces the number of the rules dropping out the non relevant rules or merging the similar rules.

The methods following the second way produce a rule base directly that does not cover fully the antecedent space. Usually they follow one of the following four approaches.

1) Try to identify the so-called optimal fuzzy rules (e.g. [29]).

2) Extend the rule base by applying the concept of Rule Base Extension (e.g. [30]).

3) Create the starting rules based on fuzzy clustering (e.g. [31]).

4) Apply evolutionary algorithms (e.g. [32],[33]) for the identification of the parameters.

C. RBE-DSS

The rule base extension using default set shapes (RBE-DSS) [30] proved to be a useful tool for the solution of fuzzy model identification problems when the model should be generated based on input-output data directly generated from the underlying process. It suggests the creation of a fuzzy system in two steps. In the first step one defines the first two rules and initiates the rule base with them. These relations describe the typical minimal and maximal outputs. For this one looks for the two output extremes and then searches the typical data rows for them. If more data rows contain the same minimum/maximum output that one is chosen which is closer to the border of the antecedent field.

Next one assigns fuzzy sets to the data using trapezoidal fuzzyfication with predefined core and support width values (default set shapes). The reference points of the resulting linguistic terms coincide with the values of the two data rows.

The RBE concept extends the rule base in course of an iterative process. In each iteration cycle it tunes the parameters of the rule set using a heuristic hill climbing approach. Each parameter is modified one by one in both of the possible upper and lower (increasing and decreasing) directions. After determining a new value for the current parameter the system is evaluated calculating the actual value of the performance index (e.g. root mean square of the error). If this is better than the previous minimum the new parameter value is kept.

The amount of modification of the set parameters depends on the range of the current input/output dimension, i.e. the step is calculated by multiplying the range by a coefficient. The iteration starts with a prescribed value of the coefficient. If the improvement of the system slows down or even stops, i.e. the value of the performance index does not improve more than a prescribed threshold during one iteration cycle; the coefficient is divided by two unless its

TABLE I.
PERFORMANCE OF THE FUZZY MODELS

	CIS	YS
RMSEP	2.1594 %	0.4795 %

vale is already equal to the allowed minimum. In that case one generates a new rule.

Each 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-DSS uses default set shapes (typical for each partition) for the determination of the shape of the new sets. These default values are identical to those used for the generation of the first two rules.

V. RESULTS AND DISCUSSION

In this study, two fuzzy models have been developed to predict the Charpy impact strength (CIS) and 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 nanotube, the ABS, and the PC the models use only two of them (nanotube and ABS) as input variables because the percent amount of the PC is a dependent variable.

We used the root mean square of the error expressed in percentage of the output variable's range (RMSEP) as performance measure of the fuzzy models. The first fuzzy system developed for CIS prediction contains 24 rules, the second model generated for YS contains 30 rules for the description of the relation between the input and output. In both cases the rule base is sparse. The application of sparse rule base targeting techniques resulted in a notable size reduction of the rule base compared to the case of the full coverage. The cut was 27.27 % in case of the CIS model and 31.82 % in case of the YS model. Figures 5 and 6 illustrate the two rule sets. Each rule is represented by a brick defined by the supports of the fuzzy sets contained in the rules.

The performance of the system is characterized in Table I. Figures 7 and 8 give a qualitative view of the model evaluation. Both systems have two input dimensions; therefore the measured and calculated output values can be visualized only by 2D plots where the horizontal axis represents the ordinal number of data points. One can observe clearly that the results calculated by the fuzzy model give a good approximation of the data originated from the experiment.

VI. CONCLUSIONS

The paper presented the application of RBE-DSS rule base identification and LESFRI fuzzy rule inference methods for fuzzy modeling of the relation between the mechanical properties of the thermoplastic composites and the percent amount of their components. The models were evaluated using RMSEP as performance indicator. Conform the testing results the two generated models proved to be good predictors of the studied process.

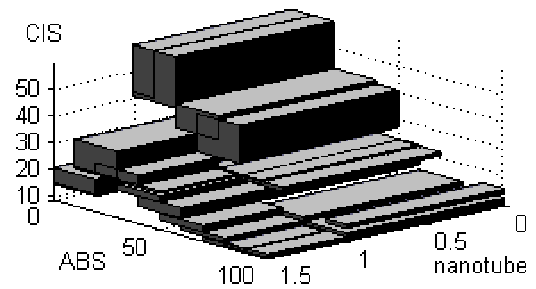

Fig. 5. Rule base of the fuzzy model describing the relation between Charpy impact strength (CIS) and the nanotube and ABS amount

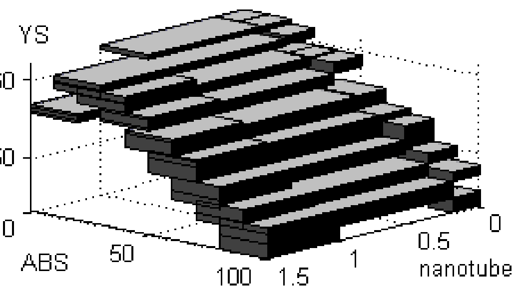

Figure 6. Rule base of the fuzzy model describing the relation between Yield strength (YS) and the nanotube and ABS amount

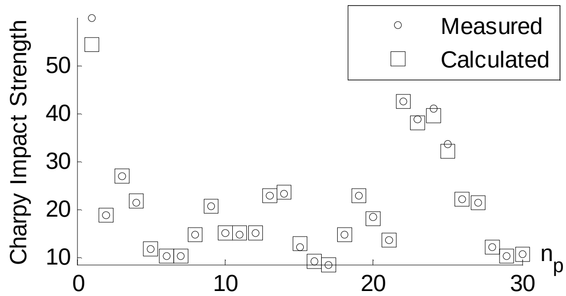

Figure 7. Measured and calculated values in case of the Charpy impact strength (CIS) model

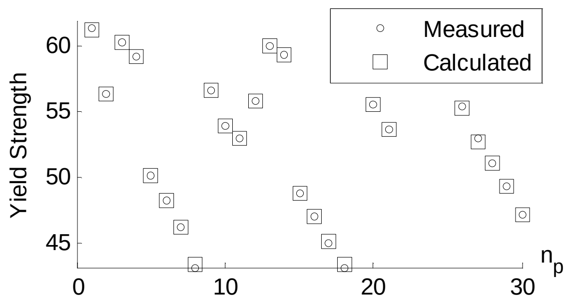

Figure 8. Measured and calculated values in case of the Yield strength (YS) model

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