

FUZZY MODELING OF THERMOPLASTIC COMPOSITES' MELT VOLUME RATE

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Abstract. Melt volume-flow rate (MVR) is one of the most important quality indicators of composite materials, which depends on the proportion of the component materials. This paper reports the development of a low complexity fuzzy model that describes the relation between percentage amount of multiwall carbon nanotube (MWCNT), acrylonitrile-butadiene-styrene (ABS), polycarbonate (PC) and MVR of the resulting composite. The rule base was generated from a sample data set obtained from experiments by the rule base extension using default set shapes (RBE-DSS) method, and the applied fuzzy inference technique was the least squares method based fuzzy rule interpolation (LESFRI). The resulting model was validated against a separate test data set as well, and it was compared to a fuzzy model generated by a traditional commercial software tool.

Keywords: Melt volume rate, fuzzy modeling, LESFRI, RBE-DSS

Mathematics Subject Classification 2010: 68T37, 03B52, 03E72

1 INTRODUCTION

Thermoplastic composites are between the most widely used material groups. Their popularity originates from their advantageous mechanical properties, thermal stability, fire resistance, etc. that are related to the proportion of the component materials [1].

One of the important indicators of the thermoplastics' quality is the melt volume-flow rate (MVR). Our research aimed at creation of a model that describes the relation between the proportion of the component materials and MVR in case of certain composites in order to make possible the prediction of MVR values in case of other amounts of components previously not tried through practical experiments.

Methods belonging to the family of computational intelligence techniques have gained a large application area in diverse fields. For example, successful solutions have been reported in [3] in fuzzy modeling based image retrieval, in [10] in misfire detection in automobile engines, in [12] in multi-robot control systems for pursuit-evasion problem, in [21] in modeling behavior-based control structures, in [17] in creating models for an anaerobic tapered fluidized bed reactor, in [24] in supporting the reliability analysis in automotive engineering, and in [25] in fuzzy control. Owing to its good interpretable knowledge representation (in form of rules) we chose fuzzy rule based systems to model the studied phenomena.

The rest of this paper is organized as follows. Section 2 gives a short introduction to MVR measurement. Section 3 recalls the key ideas of the method used for automatic rule base generation. Section 4 presents the applied fuzzy inference method. Section 5 reports the results of the model building, and finally the conclusions are drawn in Section 6.

2 MELT VOLUME-FLOW RATE

The melt flow properties of thermoplastics are non-Newtonian [8], i.e. they flow easier when the melt is at high temperature and fast injection speed during the melting process. The melt volume-flow rate (MVR) is a widely used indicator of the manner in which a polymer flows at a particular shear stress and temperature. The MVR is calculated as the volume of a polymer melt that is extruded in 10 minutes under the effect of a defined force and temperature through a standard die. Its determination methodology is defined in the standards ISO 1133:2005 [13] and ASTM D1238-10 [4] and it is sketched in Figure 1.

3 AUTOMATIC RULE BASE GENERATION WITH RBE-DSS

Automatic fuzzy rule base generation aims at creation of a fuzzy rule base from a sample data set that describes cohesive input-output value tuples originated usually from planned experiments or observations. In ideal cases the sample should give a good description of the modeled phenomena, e.g. minimum-maximum values, inflexion points, etc.

Basically there are two main trends in automatic rule base generation. The first one divides the task into two separate steps, i.e. structure definition and parameter optimization. For example, the results reported in [26, 7, 6] belong here.

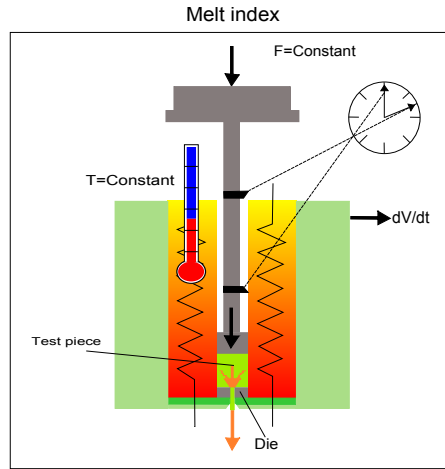


Fig. 1. Melt volume rate determination [22]

The second trend 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. [16, 29]).

In this case the rule base extension with default set shapes (RBE-DSS) method [16] was chosen owing to the fact that usually it produces a low complexity rule base with a reduced number of rules. The key idea of the rule base extension (RBE) is that it starts with the creation of two rules, describing the maximum and minimum output, respectively. When several data tuples (with different input values) contain the same extreme output value, that one which is closer to the bounds of the antecedent space is chosen.

Having the position of the initial rules the default set shapes, i.e. the shape types (e.g. trapezoidal, triangular, Gaussian, etc.) and the shape parameters are defined. For example if trapezoidal type is chosen, the width values of the support and core will be the parameters supposing that “core centre” type reference point and symmetric shape is used. These values are calculated multiplying the range of the current dimension by predefined constants.

After defining the initial rules a tuning algorithm is started whose algorithm is presented in Figure 2.

The initial step (s_0), the maximum number of iteration cycles (i_{max}), the minimum allowed step size (s_{min}), and the target (prescribed) performance index (PI_{pr}) are parameters of the method. The performance of the system is evaluated by the root mean square of the error (RMSE) or by RMSE expressed in percentage of the output range (RMSEP).

The key idea of the method is that in each iteration cycle for each parameter (p) two new values are calculated, one by decreasing it by s and one by increasing it by s . The system is evaluated for each value and that one, which ensures the best

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s ← s0
PI0 ← Evaluate initial system
PIbest ← PI0
for i = 1 → imax do
  for each antecedent and consequent dimension do
    for each fuzzy set do
      for each parameter do
        for both possible directions do
          p ← Calculate new parameter value
          PI ← Evaluate system
          if PI < PIbest then
            Store p
            PIbest ← PI
            if PIbest < PIpr then
              STOP
            end if
          end if
        end for
      end for
    end for
  end for
   $\Delta PI \leftarrow |PI_0 - PI_{best}|$ 
  PI0 ← PIbest
  if  $\Delta PI < \Delta PI_{min}$  then
    s ← s/2
    if s < smin then
      Create new rule
      s ← s0
    end if
  end if
end for

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Fig. 2. RBE-DSS algorithm

system performance (PI) is kept. When the amelioration of PI in course of two consecutive iterations slows down or stops, the step is halved. When the step size becomes too small ($s < s_{min}$), a new rule is created.

In order to create the new rule, that calculated data point which differs most from its corresponding training point is sought. The input and output values of this training point will be used as reference points for the antecedent and consequent sets of the new rule. These sets are created using the default set shapes.

The algorithm stops either when the maximum allowed iteration cycle number is reached or the system performance becomes better than the target performance index (PI_{tr}). The method is implemented in the SFMI toolbox [14].

4 FUZZY INFERENCE

Application of the above presented RBE concept usually leads to a sparse rule base, i.e. a rule base where some parts of the input space are not covered by rule antecedents. Therefore such a fuzzy inference method is needed that ensures a valid and proper conclusion even in those regions of the input space where none of the known rules can be fired. The applicable methods do the reasoning by the means of an interpolation between the available rules.

There are several fuzzy rule interpolation (FRI) techniques (e.g. [9, 11, 19, 20, 23, 28, 30]). In this case the LESFRI [15] was chosen owing to good previous experiences and to the fact that being implemented in the FRI toolbox [18] it was freely available.

The least squares method based fuzzy rule interpolation (LESFRI) follows the concept of the generalized methodology of fuzzy rule interpolation [5] by inferring the conclusion in two steps. Firstly, it creates a new rule in the position defined by the reference points of the observation (input) sets. Secondly, it produces the conclusion using the single rule reasoning SURE-LS [15].

In the first step the calculations are done separately in each antecedent dimension by the means of the set interpolation technique FEAT-LS [15]. It applies the concept of linguistic term shifting, i.e. each known antecedent set of the current dimension is virtually shifted into the position of the observation's reference point in the current dimension (see Figures 3 and 4). Next, the characteristic points of the new set shape result from a calculation based on the method of weighted least squares, which takes into consideration the corresponding characteristic points of the overlapped set shapes weighted by their original distance from the interpolation point. The calculations are done α -cut-wise.

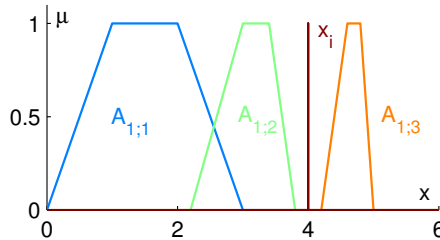


Fig. 3. Original sparse partition in the first antecedent dimension with three known fuzzy sets and the x_i interpolation point

LESFRI determines the position of the new rule's consequent set by applying an extended version of the classical crisp Shepard interpolation [27]. The shape of the consequent set is determined by the single rule reasoning method SURE-LS [15], which does the calculations α -cut-wise as well. In each antecedent dimension in case of each α -cut it measures the differences between the endpoints of the antecedent

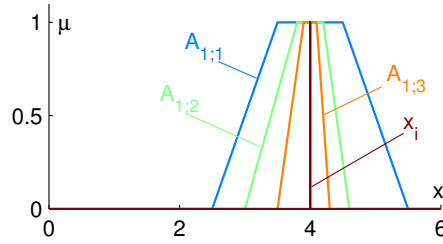


Fig. 4. Virtually shifted fuzzy sets and the x_i interpolation point

set’s α -cuts and the observation set’s α -cuts. Next, it calculates the α -cuts of the conclusion by modifying the α -cuts of the rule consequent with the average of the distances measured in the individual dimensions.

The final set shape is determined from the α -cut endpoints by calculating the parameters of the selected set shape type (e.g. trapezoidal, triangular, singleton) using the least squares method.

5 RESULTS

The purpose of our research was to create a low complexity fuzzy model, which describes the relation between the MVR and the percent amount of the components in thermoplastic composite production. Although the mixture contained three components, namely multiwall carbon nanotube (MWCNT), acrylonitrile-butadiene-styrene (ABS), and polycarbonate (PC), the model uses only two of them (MWCNT and ABS) owing to the percentage relation

$$MWCNT + ABS + PC = 100 \%, \tag{1}$$

which expresses that PC is a dependent variable.

The sample data contained the results of 24 experimental setups [2]. Each setup was carried out with 10 replications, which results in the total of 240 experiments. The experimental results were divided 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 18 experimental setups (180 experiments). The testing data set contained the results of 6 experimental setups (60 experiments).

The performance of the resulting fuzzy system was measured using the root mean squared error expressed in percentage of the output variable’s range (RMSEP). It was chosen because it facilitates the interpretation of the error and its benchmarking against the width of the variation interval of the output. Figure 5 presents the rule antecedents of the starting rule base. In accordance with the RBE concept the initial rule base contains only two rules: one for the selected minimum output and one for the selected maximum output.

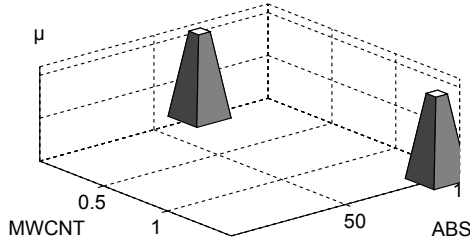


Fig. 5. Rule antecedents of the starting fuzzy system

Tuning of a fuzzy system based on a sample data set can easily lead to an “over-fitting”, i.e. the output of the system is very close to or quite identical with the output of the modeled phenomena in case of the sample training data; however, it differs considerably from the modeled phenomena in case of other input values.

In order to avoid this dead-end the performance of the system was also measured against the test data in case of each potential parameter tuple, i.e. in course of each iteration cycle. Figure 6 presents the variation of the fuzzy system performance in function of the number of iteration cycles (tuning) in case of the training data (PI_{tr}) and in case of the testing data (PI_{te}).

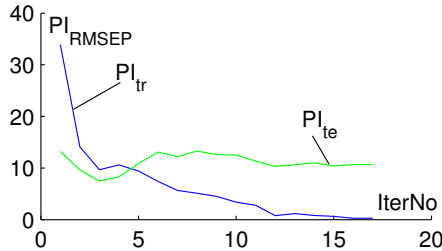


Fig. 6. Performance variation of the fuzzy system in course of tuning in case of the training data (PI_{tr}) and in case of the testing data (PI_{te})

Surprisingly at the beginning for several iteration cycles the generated parameter tuples ensure a better performance in case of the test data set (PI_{te}). However, in parallel with the improvement of PI_{tr} a performance decay can be observed in case of PI_{te} followed by a quasi stabilization at about 10.5% while PI_{tr} reaches the value of 0.28%, which is a clear sign of overfitting.

Owing to the RBE approach the number of the rules increases continuously (see Figure 7) in the course of tuning which also increases the complexity of the fuzzy system.

In order to satisfy all the requirements, namely good performance against the training and testing data sets as well as a reduced number of rules (low system

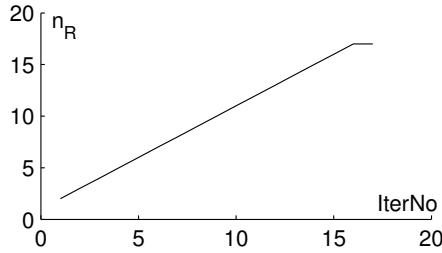


Fig. 7. Variation of the rule number (n_R) in the course of tuning

complexity), we enhanced the original RBE-DSS method by creating an overall evaluation index (E) that takes into consideration all the above-mentioned factors. In case of the i^{th} iteration its value is determined by

$$E^i = \frac{\frac{PI_{tr}^i \cdot n_{tr} + PI_{te}^i \cdot n_{te}}{100 \cdot (n_{tr} + n_{te})} \cdot w_{PI} + \frac{n_R^i}{n_{Rmax}} \cdot w_R}{w_{PI} + w_R}, \tag{2}$$

where n_{tr} and n_{te} are the numbers of the data points in the training and test data sets, w_{PI} and w_R are the weights associated to the performance index and the rule number, n_R^i is the number of rules, and n_{Rmax} is the maximum rule number (encountered at the end of the tuning). The first component of the numerator is divided by 100 because the original performance values (PI_{xx}) are expressed in percentage. In our case the weighted average of the performance values was much more important than the number of the rules. Therefore the weights $w_{PI} = 0.9$ and $w_R = 0.1$ were used in the course of calculations.

Similar to PI , the measure E is of type “the smaller the better”, i.e. the parameter tuple that ensures the minimum value of E is kept. Figure 8 shows the variation of E in function of the number of iteration cycles. Table 1 summarizes the values of the overall evaluation index and its components in case of some important iteration cycle numbers, i.e. the lowest rule number ($IterNo = 1$), the smallest PI_{te} value ($IterNo = 3$), the best E value ($IterNo = 12$), and the smallest PI_{tr} value ($IterNo = 16$).

$IterNo$	PI_{tr}	PI_{te}	n_R	E
1	33.9157	13.2203	2	0.2704
3	9.6667	7.4957	4	0.1056
12	0.7886	10.3270	13	0.1050
16	0.2767	10.6631	17	0.1259

Table 1. The values of the overall evaluation index and its components in case of some important iteration cycle numbers

Taking into consideration the above aspects we chose the fuzzy model (parameter tuple) produced in the course of the 12th iteration cycle. The antecedent space and

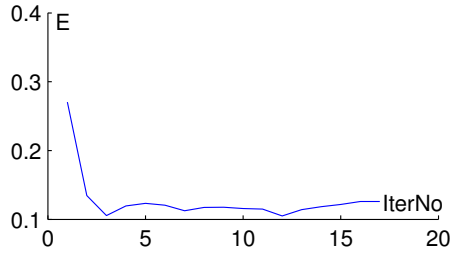


Fig. 8. Variation of the overall evaluation index of the fuzzy system in the course of tuning

the rule base of the resulting system are presented in Figures 9 and 10. In general, the used fuzzy sets are trapezoid-shaped; however, in some cases their shape can degenerate to a singleton form.

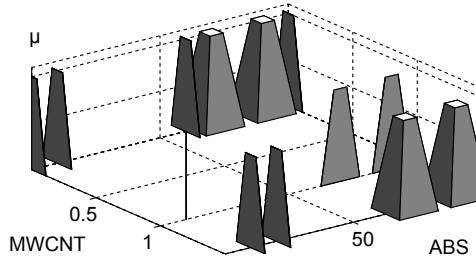


Fig. 9. Rule antecedents of the final fuzzy system

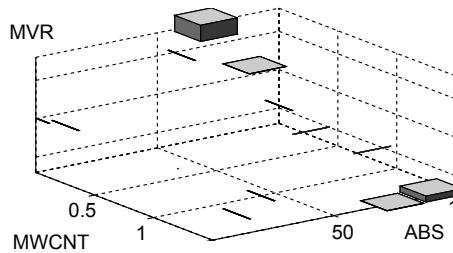


Fig. 10. Rules of the final fuzzy system

In Figure 10 each rule is represented by a brick whose edges are defined by the supports of the rule antecedent and consequent sets.

As a final control of the results we also tried a well known commercial product, the ANFIS software of the Matlab's Fuzzy Logic ToolBox. In this case the

starting fuzzy system was created based on a grid partitioning of the input universe using five trapezoid shaped fuzzy sets in each input dimension. The type of the output membership functions was constant and the applied inference technique was of Takagi-Sugeno type. We used the hybrid training method with five epochs and zero error tolerance. The training and testing data sets were identical with those used previously.

The resulting average training and testing error values were 0.6633 and 1.7375, respectively. Table 2 contains the performance values expressed in RMSEP, the number of the rules and the overall evaluation index in case of the ANFIS based solution. It can be recognized clearly that the above RBE-DSS and LESFRI based solution ensured a better E value.

PI_{tr}	PI_{te}	n_R	E
4.7181	12.3584	25	0.1597

Table 2. The value of the overall evaluation index and its components in case of the solution created by the ANFIS software

6 CONCLUSIONS

The paper reported fuzzy modeling of the relation between the percentage of the components and the melt volume-flow rate of MWCNT-ABS-PC composite materials. The rule base was generated by the RBE-DSS method and LESFRI was used as fuzzy inference technique. An enhancement of the original RBE-DSS method was also presented, which makes possible taking into consideration the performance of the system in a weighted form against both the training and testing data as well as the number of the rules.

In the course of iterative tuning several models were created from which that one was chosen, which ensured the best overall evaluation index. It took into consideration in a weighted manner the performance against the training and test data as well as the number of the rules. The resulting fuzzy system can be used to predict the MVR value in function of the components' amount. Finally, the performance of the created fuzzy system was compared to the performance of a fuzzy system generated by the ANFIS software using the same training and test data sets. In case of all the main components of the applied overall evaluation index our fuzzy system ensured better results than the the system created by ANFIS.

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