Fibers and Polymers 2006, Vol.7, No.4, 404-413

Optimization of Multiple Quality Characteristics for Polyether Ether Ketone Injection Molding Process

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(Received June 29, 2006; Revised November 8, 2006; Accepted November 14, 2006)

Abstract: This study examines multiple quality optimization of the injection molding for Polyether Ether Ketone (PEEK). It also looks into the dimensional deviation and strength of screws that are reduced and improved for the molding quality, respectively. This study applies the Taguchi method to cut down on the number of experiments and combines grey relational analysis to determine the optimal processing parameters for multiple quality characteristics. The quality characteristics of this experiment are the screws' outer diameter, tensile strength and twisting strength. First, one should determine the processing parameters that may affect the injection molding with the $L_{18}(2^1 \times 3^7)$ orthogonal, including mold temperature, pre-plasticity amount, injection pressure, injection speed, screw speed, packing pressure, packing time and cooling time. Then, the grey relational analysis, whose response table and response graph indicate the optimum processing parameters for multiple quality characteristics, is applied to resolve this drawback. The Taguchi method only takes a single quality characteristic into consideration. Finally, a processing parameter prediction system is established by using the back-propagation neural network. The percentage errors all fall within 2 %, between the predicted values and the target values. This reveals that the prediction system established in this study produces excellent results.

Keywords: Polyether ether ketone, Injection molding, Taguchi method, Grey relational analysis, Neural network

Introduction

PEEK is a semi-crystalline thermoplastic polymer (typically 35 %) with outstanding characteristics, such as excellent mechanical properties, high melting point and good resistance to strong acids. It has more wide-ranging applications than most polymers. The high performance PEEK polymer was first prepared by Bonner in 1962 [1]. He synthesized the poly (aryl-ether-ketone) with the solvent dephenylsulfone and carried out the substitution reaction of aromatics at melting point of the polymer [2]. Most standard reciprocating screw injection molding machines are capable of molding PEEK polymer and compounds. Complex high performance components can be readily mass-produced without the need for annealing or conventional machining. PEEK polymer and compounds based on PEEK polymer can be readily injection molded. However, due to the high melting temperature, certain design and process variables need to be considered. The configuration of the processing parameters for the injection molding process is the focus since an optimal processing parameters design could help solve most quality-control problems.

The processing parameters that may affect an injection molding process include the following: mold temperature, pre-plasticity amount, injection pressure, injection speed, screw speed, packing speed, packing pressure, packing time and cooling time, etc. [3-8]. The adjustment of the processing parameters is often done considering the mold cavity design and its size, the properties of plastic materials and the defects of the molding product, etc. Such tasks require accumulated data and experience from a large number of tests and experiments to clarify the causes of product defects. They also entail a time-and effort-consuming process.

Based on the reasons mentioned above, Chang *et al.* [9] adopted the Taguchi method for the processing parameter design of the injection molding to reduce shrinkage in the molded product. Results from experiments showed that the optimal conditions to effectively reduce shrinkage in the product can be achieved by using the Taguchi method. However, this method focused on a single quality characteristic, whereas the actual production process involved more than one quality characteristic. The relationship between multiple quality characteristics and processing parameters was not taken into consideration in optimizing a single quality characteristic. Moreover, there may be some inconsistencies among the different designs for various single quality characteristics, in which case the adjusted processing parameters were unlikely to be optimum ones. In response to this problem, Lin *et al.* [10] applied the grey relational analysis in combination with the Taguchi method to the optimization of the processing parameters for the electrical discharge machining process. The optimum processing parameters were obtained after the orthogonal array experiments and after applying the grey relational analysis on the experimental data. The experimental results proved the effectiveness of process quality improvements in their study. In addition, Yousef *et al.* [11] applied the neural network to the non-linear laser micro-machining process and predicted the level of pulse energy needed to produce a dent or a crater with the desired depth and diameter. Their experimental results proved that the neural network was able to predict the behavior of the material removal process with a high accuracy.

In view of the above researches, this study planned to

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adopt the Taguchi method for the experiment with the screw's outer diameter, tensile strength and twisting strength as the quality characteristics. Next, an appropriate orthogonal array was selected to conduct the experiment. The grey relational analysis was then applied to identify the optimum processing conditions for multiple quality characteristics of the molded screw. The significant factors that affected the quality characteristics could be obtained through an analysis of variance (ANOVA), which would in turn be used to infer and to confirm the confidence interval for the experiments and to verify the reproducibility of these factors. In addition, the non-linear correlation model between the process parameters and the screw's outer diameter, tensile strength and twisting strength would be established by BPNN using experimental results from the orthogonal array as training sets and test sets. This is done in order to establish a quality prediction system for PEEK injection molding. The flowchart of the experimental process is shown in Figure 1.

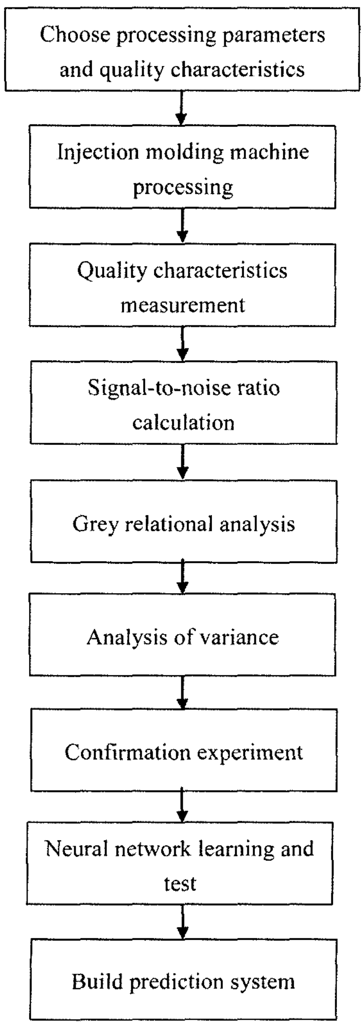

Figure 1. Flowchart of the experimental process.

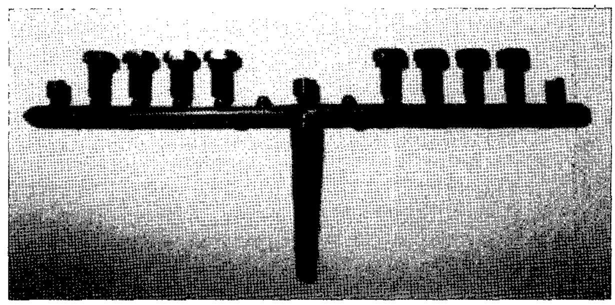

Figure 2. The hexagonal screw.

Experimental Materials and Equipment

The materials used for injection molding are: Polyether Ether Ketone (PEEK), serial no. 450G produced by VICTREX Co., Ltd.. PEEK polymer is a linear aromatic semi-crystalline thermoplastic. The materials were placed in an air circulating oven for minimum of three hours at 150 °C in order to achieve successful molding. The powder and granules were dried to less than 0.1 % w/w moisture. The injection molding machine used for the experiment is the 270S 250-60, made by ARBURG Co., Ltd. The injection molded hexagonal screw is shown in Figure 2. Tensile and twisting strength of hexagonal screws were tested with a Tensilon RTA-1T, made by Orientec Corp.

Research Method

Taguchi Quality Method

This study applied the Taguchi method [12-14] to plan the PEEK injection molding experiments. An appropriate orthogonal array was chosen in accordance with the control factors and their levels in order to identify optimal PEEK injection molding quality with the minimum number of experiments late. At the same time the experiments still maintained the robustness in the process.

The $L_{18}(2^1 \times 3^7)$ orthogonal array, which represented eighteen sets of experiments and contained one two-level factor and seven three-level factors, was selected for this study. Since this study sought to achieve outer diameter of 4.066 mm for the screws. The greater the tensile and twisting strengths, the better. The quality characteristics for the screw's outer diameter as well as its tensile strength and twisting strength therefore belonged to the nominal-the-better and the larger-the-better categories, respectively. The signal-to-noise ratios (SN ratios) for the nominal-the-better and the larger-the-better are respectively shown as follows:

$$SN = 10 \log \frac{u^2}{\sigma^2} \tag{1}$$

where u stands for the mean value of the observed value, and σ represents the standard deviation of the experiment samples.

$$\mathrm{SN} = -10\log\frac{1}{n}\sum_{i=1}^{n}\frac{1}{y_i^2} \quad (2)$$

where y_i stands for the observed value in the experiment, and n represents the total observed numbers.

Main Effect Analysis

According to the orthogonal array, the experimental data could be obtained after conducting the experiments. When the data were calculated for the SN ratios, the response table and the response graph would be established. The mean response value $\overline{F_i}$ for each factor levels was obtained first, followed by the main effect value ΔF for each factor levels. Next, the response table and response graph could be acquired from this data and the effect analysis of the factors was computed. The higher a factor's main effect value, the greater this factor's impact on the system will be when compared to the other factors. The method of calculation is as follows:

$$\overline{F_i} = \frac{1}{m}\sum_{j=1}^{m}y_{ij} \quad (3)$$

$$\Delta F = \max(\overline{F_1}, \overline{F_2}, \ldots, \overline{F_n}) - \min(\overline{F_1}, \overline{F_2}, \ldots, \overline{F_n}) \quad (4)$$

where $\overline{F_i}$ is the mean SN ratio of the ith level of factor F, m is the number of the ith level of each factor, y_{ij} is the jth SN ratio of the ith level, ΔF is the value of the main effects of factor F, and n is the number of the level of each factor.

Analysis of Variance

ANOVA was used to evaluate the experimental error and significance test. This application of statistical testing on factors helps to identify the effects of the individual factors. The use of the F test compensates for the defects of the Taguchi method experiments, such as failure to identify the effects that the different experiments may have on quality characteristics or the level of experimental errors.

Experimental Error Estimation

The degree of freedom (DOF) must be determined for each control factor before ANOVA can be conducted. The DOF was defined as:

$$\mathrm{DOF} = r - 1 \quad (5)$$

where r stands for the number of repeated experiments.

The definition of errors in each factor experiment is as follows:

$$S = \sqrt{\frac{\sum(y_i - \overline{y})^2}{DOF_{Error}}} \quad (6)$$

where S stands for the mean variance of each factor, y_i represents the experiment value for each time, $\overline{y}$ is the mean value in the experiment, and DOF_{Error} is the degree of freedom error (DFE).

Response value, also called sum of square (SS), stands for the response value of the individual factor level in response to factor variance, the equation of which is as follows:

$$SS_{Factor} = \frac{n \times r}{L}\sum_{k=1}^{L}(\overline{y}_k - \overline{y})^2 \quad (7)$$

$$DOF_{Factor} = L - 1 \quad (8)$$

where "Factor" represents the name of the individual factors, n is the number of experiments, and L is the number of each factor level.

The definition of the total experimental error is as follows:

$$SS_{Factor} = \sum_{i=1}^{n}S^2 \times (r-1) \quad (9)$$

$$DOF_{Factor} = n \times (r-1) \quad (10)$$

$$S = \sqrt{\frac{SS_{Error}}{DOF_{Error}}} \quad (11)$$

The total experimental error represents the sum of all variances between experimental errors and all factors, i.e. $SS_{Total} = SS_{Factor} + SS_{Error}$.

Factor Significance Test

The F test examines the relationships between the variances generated from the experimental errors in the experiments and the variances of individual factors. It can be conducted to examine the significant factors. The definition of F test is:

$$F = \frac{mS_{Factor}^2}{S^2} \quad (12)$$

where m represents the number of repeated experiments.

The F test clearly shows that the variance of this factor has a significant effect on the experiments and that this factor should not be ignored.

Confirmation Experiment

The main purpose of this experiment was to verify whether the conclusion obtained from the analysis of experiment data was correct. The SN ratio under optimum conditions could be inferred by using an addition mode. The calculation thereof is as follows:

$$\hat{SN} = \overline{T} + \sum_{i=1}^{n}(F_i - \overline{T}) \quad (13)$$

where n is the number of the significant processing parameters, $\overline{T}$ is the total average of the SN ratios in the experiments and F_i is the mean response value of the ith level of the significant processing parameters.

To effectively evaluate all the values observed, the confidence intervals thereof must be calculated. The mean value expected was chosen for this study, the equation of which is as follows:

$$CI = \sqrt{F_{\alpha,1,\nu_2} \times V_e \times \left(\frac{1}{n_{eff}} + \frac{1}{r}\right)} \tag{14}$$

where $F_{\alpha,1,\nu_2}$ is the tabulated F-ratio, α is the risk (confidence level = $1-\alpha$), ν_2 is the degree of freedom for the numerator associated with the pooled error variance. V_e is the pooled error variance, r is the sample size ($r \neq 0$), and n_{eff} is the effective number of experimental observations and calculated as

$$n_{eff} = \frac{\text{total number of experiments}}{\text{sum of degrees of freedom used in estimate of mean}} \tag{15}$$

The 95 % confidence intervals which have 0.95 probabilities of containing the parameter are used, the equation of which is as follows:

$$\hat{S}N - CI \leq \mu_{confirmation} \leq \hat{S}N + CI \tag{16}$$

In the equation, $\mu_{confirmation}$ stands for the actual mean value in the confirmation experiment.

Grey Relational Analysis

The Taguchi method was used mostly to optimize the single quality characteristic. The optimum processing parameters that determined a single quality characteristic, however, often failed to represent a processing parameter optimization of the overall quality. Therefore, the grey relational analysis was adopted for this study to compare the relational grades between the reference sequence $x_0(k)$ and the comparative sequences of $x_1(k), x_2(k), \ldots, x_m(k)$.

Among these, the reference sequence stands for the target value of the hexagonal screw's outer diameter as well as the maximum mean values of the tensile and twisting strength obtained from the L_{18} orthogonal array experiments, that is, $X_0 = (4.066, 842.8, 0.599)$ The comparative sequences were the quality characteristics obtained from the L_{18} orthogonal array experiments.

The calculation steps for the grey relational analysis are as follows [15]:

Step 1: Mean of each sequence.

$$\text{Let } X_i' = X_i/x_i(1) = (x_i'(1), x_i'(2), \ldots, x_i'(n)) \\ i = 0, 1, 2, \ldots, m \tag{17}$$

Step 2: Differential sequence.

$$\Delta_i(k) = |x_0'(k) - x_i'(k)|,\ \Delta_i = (\Delta_i(1), \Delta_i(2), \ldots, \Delta_i(n)) \\ i = 1, 2, \ldots, m \tag{18}$$

Step 3: Maximum and minimum differences of both grades.

$$M = \max_i \max_k \Delta_i(k),\quad m = \min_i \min_k \Delta_i(k) \tag{19}$$

Step 4: Grey relational coefficient.

$$\gamma_{0i}(k) = \frac{m + \zeta M}{\Delta_i(k) + \zeta},\ \zeta \in (0, 1) \\ k = 1, 2, \ldots, n;\ i = 1, 2, \ldots, m \tag{20}$$

where ζ is the distinguishing coefficient and 0.5 is adopted for this study.

Step 5: Grey relational grade.

$$\gamma = \frac{1}{n}\sum_{k=1}^{n} \gamma_{0i}(k),\ i = 1, 2, \ldots, m \tag{21}$$

When the quality characteristics of hexagonal screws were input to the reference sequence, calculations can be conducted immediately to obtain the grey relational grades with the L_{18} orthogonal array experimental data. The grey relational grades were then analyzed in the main effect analysis. The optimization of multiple quality processing parameters for the hexagonal screws can be obtained from the response graph and response table.

Back Propagation Neural Network

The basic principle of the back-propagation neural network (BPNN) is to minimize the error function by using the steepest gradient descent method. The results of twelve experiments conducted according to the L_{18} orthogonal array were taken as the training sets. Another six sets were taken as the test sets. When each learning set was entered, the network rectified the weights and biases. The BPNN established in this study has three layers, which are the input layer, hidden layer and

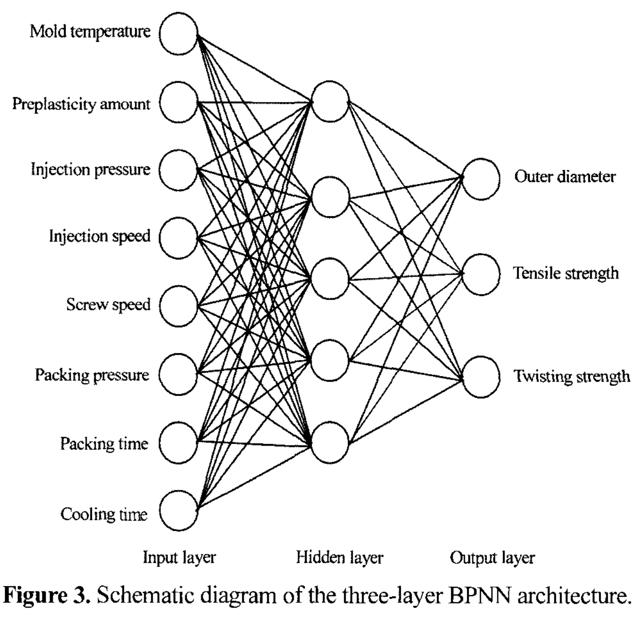

Figure 3. Schematic diagram of the three-layer BPNN architecture.

output layer. Among these layers, there are eight processing elements in the input layer, including the mold temperature, pre-plasticity amount, injection pressure, injection speed, screw speed, packing pressure, packing time and the cooling time. The processing elements in the output layer have three quality characteristics – the screw's outer diameter, tensile strength and twisting strength. The schematic diagram of the BPNN is shown in Figure 3.

The BPNN is a supervised learning network, which learns through the input training sets given the corresponding data. The purpose of the network's learning is to build the relationship between the input and output during the training process. After that, the final weights and biases can be arrived at. The output value will be close to the target value [16-18]. The criterion for the error function adopted in the network is as follows:

$$E = \frac{1}{2}\sum(T_j - Y_j)^2 \tag{22}$$

where T_j and Y_j respectively represent the target output and the predicted output of jth output neuron in the output layer.

The learning steps of the BPNN are as follows:

Step 1: Input the input vector X and target output vector T of the training sets.

Step 2: Calculate the output vector H of the hidden layer.

$$net_k = \sum_i W_{ik}X_i - \theta_k \tag{23}$$

$$H_k = f(net_j) = \frac{1}{1+e^{-net_k}} \tag{24}$$

where i stands for the number of input neurons, j stands for the number of the output neurons, k stands for the number of neurons in the hidden layer, W_{ik} stands for the weight between the input layer and the hidden layer, and θ_k stands for the bias of the hidden layers.

Step 3: Calculate the output vector Y in the output layer.

$$net_j = \sum_k W_{kj}H_k - \theta_j \tag{25}$$

$$Y_j = f(net_j) = \frac{1}{1+e^{-net_j}} \tag{26}$$

where W_{kj} stands for the weight between the hidden layer and output layer, and θ_j stands for the bias of the output layer.

Step 4: Calculate the interval scale δ.

The interval scale of the output layer is

$$\delta_j = (T_j - Y_j)\cdot f'(net_j) = (T_j - Y_j)\cdot Y_j \cdot (1 - Y_j) \tag{27}$$

The interval scale of the hidden layer is

$$\delta_k = \left(\sum_j \delta_j W_{kj}\right)\cdot f'(net_k) = H_k\cdot(1 - H_k)\cdot \sum_j \delta_j W_{kj} \tag{28}$$

Step 5: Calculate the weight correction and bias correction.

The weight correction and bias correction of the output layer are shown respectively as follows:

$$\Delta w_{kj}^n = \eta\delta_j H_k + \alpha\cdot\Delta W_{kj}^{n-1} \tag{29}$$

$$\Delta\theta_j^n = -\eta\delta_j + \alpha\cdot\Delta\theta_j^{n-1} \tag{30}$$

The weight correction and bias correction of the hidden layer are shown respectively as follows:

$$\Delta w_{ik}^n = \eta\delta_k X_i + \alpha\cdot\Delta W_{ik}^{n-1} \tag{31}$$

$$\Delta\theta_k^n = -\eta\delta_k + \alpha\cdot\Delta\theta_k^{n-1} \tag{32}$$

where η stands for the learning rate, and α stands for the momentum factor.

Step 6: Update the weights and biases.

The weights and biases in the output layer are updated respectively and shown as follows:

$$W_{kj} = W_{kj} + \Delta W_{kj} \tag{33}$$

$$\theta_j = \theta_j + \Delta\theta_j \tag{34}$$

The weights and biases in the hidden layer are updated respectively and shown as follows:

$$W_{ik} = W_{ik} + \Delta W_{ik} \tag{35}$$

$$\theta_k = \theta_k + \Delta\theta_k \tag{36}$$

Step 7: Repeat step 1 to step 6 until the error function converges.

To verify the learning results, there is a need to upload the test sets onto the network, thus completing the training work. The purpose for this is to check whether the convergence error had in fact converged into a reasonable range. Accordingly, the root-mean-square error (RMSE) was adopted as the testing method for this study, the equation of which is as follows:

$$RMSE = \sqrt{\frac{\sum_p^M\sum_j^N (T_j^p - Y_j^p)^2}{M\times N}} \tag{37}$$

where M stands for the total number of test sets, N stands for the number of neurons in the output layer, T_j^p represents the target output value of the jth output unit in the pth set, and Y_j^p represents the predicted output value of the jth output unit in the pth set.

Results and Discussion

Firstly, the screw's outer diameter, tensile strength and twisting strength were chosen as the quality characteristics. Since the maximum and minimum of the outer diameter were 4.1427 mm and 3.99 mm, respectively, the target value was set at 4.066 mm. The SN ratio of the nominal-the-better was calculated according to the equation (1). In addition, the tensile strength and twisting strength of the screws were desired, the greater, the better. Therefore, the SN ratios of the larger-the-better were calculated according to the equation (2). Then, the control factors and their levels must be chosen. The factors that can be controlled by the injection machine, the related researches in the past, and the experiences of senior engineers were considered. Afterwards, the mold trial experiments were actually conducted to facilitate the selection of an appropriate range for the processing parameters. The control factors and their levels were chosen as shown in Table 1. Based on Table 1, the control factors and their levels

Table 1. Control factors and levels

Code	Control factor	Unit	Level*		
			1	2	3
A	Mold temperature	°C	150	<u>160</u>	
B	Preplasticity amount	cm	5	6	<u>7</u>
C	Injection pressure	bar	250	450	<u>650</u>
D	Injection speed	cm/s	<u>5</u>	10	15
E	Screw speed	m/min	15	<u>20</u>	25
F	Packing pressure	bar	200	400	<u>600</u>
G	Packing time	sec	3	<u>6</u>	9
H	Cooling time	sec	<u>5</u>	10	15

*Current levels are underlined.

Table 2. The L_{18} orthogonal array layout

No.	A	B	C	D	E	F	G	H
1	150	5	250	5	15	200	3	5
2	150	5	450	10	20	400	6	10
3	150	5	650	15	25	600	9	15
4	150	6	250	5	20	400	9	15
5	150	6	450	10	25	600	3	5
6	150	6	650	15	15	200	6	10
7	150	7	250	10	15	600	6	15
8	150	7	450	15	20	200	9	5
9	150	7	650	5	25	400	3	10
10	160	5	250	15	25	400	6	5
11	160	5	450	5	15	600	9	10
12	160	5	650	10	20	200	3	15
13	160	6	250	10	25	200	9	10
14	160	6	450	15	15	400	3	15
15	160	6	650	5	20	600	6	5
16	160	7	250	15	20	600	3	10
17	160	7	450	5	25	200	6	15
18	160	7	650	10	15	400	9	5

were applied to the $L_{18}(2^1 \times 3^7)$ orthogonal array, as shown in Table 2, to create an experiment plan. Eighteen experiments were conducted in accordance with the experiment plan with each experiment repeated ten times. The experimental data subsequently were calculated into SN ratios. The averages obtained in the experiments and the SN ratios are listed in Table 3.

Then, the grey relational analysis was applied to obtain the optimum processing conditions for multiple quality characteristics. The target value of the hexagonal screw's outer diameter and the maximum mean values of the tensile strength and twisting strength of L_{18} orthogonal array were used for the reference sequence, i.e., $X_0 = (4.066, 842.8, 0.599)$. The calculation results of the differential sequence, the grey relational coefficients and grades in each experiment in the reference sequence and orthogonal array are shown in Table 4. The response table and the response graph of grey relational analysis are shown in Table 5 and Figure 4, respectively. From the response table and the response graph, the optimal processing conditions of the PEEK injection molding for the hexagonal screw was: A2, B1, C1, D3, E3, F3, G1 and H3, that is, with the mold temperature at 160 °C, pre-plasticity amount of 5 cm, injection pressure of 250 bar, injection speed of 15 cm/sec, screw speed of 25 m/min, packing pressure of 600 bar, packing time of 3 sec and a cooling time of 15 sec. With only a single quality characteristic, the screw's outer diameter, was taken into consideration, the optimum processing conditions were A2, B2, C2, D3, E3, F2, G3 and H1, that is, with the mold temperature at 160 °C, pre-plasticity amount of 6 cm, injection pressure of 450 bar, injection speed of 15 cm/sec, screw speed of 25 m/min, packing pressure of 400 bar, packing time of 9 sec and a cooling time of 5 sec.

Next, the five confirmation experiments were conducted to verify reproducibility of the factor effects. The ANOVA table, as shown in Table 6, was obtained after calculating the SN ratios of Table 3. It was clear in the ANOVA table that the control factors A, F, G, and H had a smaller effect on the outer diameter of the hexagonal screws. Hence, they were listed as pooled errors. The control factors B, C, D, and E, on the contrary, had a greater effect, and thus, were significant factors. Among them, the control factor C, the injection pressure, had the greatest effect on the outer diameter of the hexagonal screws. The significant factors of tensile and twisting strengths of the hexagonal screws were respectively A, B, C, and H as well as C, D, F, and H. The most significant factors were the mold temperature and the cooling time, respectively. According to the significant factors, it can be inferred that the expected SN ratios in the experiment fall within the 95 % confidence interval by equations (13), (14), and (16).

The 95 % confidence interval of the hexagonal screw's outer diameter, tensile strength, and twisting strength were respectively $42.0468 < \mu_{\text{diameter}} < 56.2668$, $57.7681 < \mu_{\text{tensile}}$

Table 3. The averages and SN ratios of the screw's outer diameter, tensile strength and twisting strength

Experiment no.	Diameter (mm)	Tensile (N)	Twisting (N·m)	SN ratio of diameter (dB)	SN ratio of tensile strength (dB)	SN ratio of twisting strength (dB)
1	3.943	828.1042	0.543	29.232	58.3617	−5.304
2	4.017	783.9981	0.517	36.791	57.8863	−5.7302
3	4.042	837.8958	0.559	42.483	58.4638	−5.0518
4	3.902	823.1993	0.571	34.23	58.3101	−4.8673
5	4.088	818.3046	0.484	43.673	58.2583	−6.3031
6	4.067	803.6001	0.537	43.167	58.1008	−5.4005
7	3.848	818.3046	0.556	28.143	58.2583	−5.0985
8	4.075	774.2033	0.487	42.349	57.7771	−6.2494
9	4.077	793.798	0.519	43.471	57.9942	−5.6967
10	3.993	828.1042	0.562	40.261	58.3617	−5.0053
11	4.016	813.4016	0.453	39.34	58.2061	−6.878
12	3.989	818.3046	0.495	32.891	58.2583	−6.1079
13	3.994	828.1042	0.508	37.386	58.3617	−5.8827
14	4.076	842.8009	0.599	44.281	58.5145	−4.4515
15	4.06	823.1993	0.511	41.437	58.3101	−5.8316
16	4.017	828.1042	0.537	37.291	58.3617	−5.4005
17	4.068	813.4016	0.545	42.314	58.2061	−5.2721
18	4.062	808.5	0.549	43.818	58.1536	−5.2086

Table 4. The differential sequences, grey relational co-efficients and grades

No.	$\Delta_{0,i}(1)$	$\Delta_{0,i}(2)$	$\Delta_{0,i}(3)$	$\gamma_{0,i}(1)$	$\gamma_{0,i}(2)$	$\gamma_{0,i}(3)$	$\gamma_{0,i}$
1	0	2.7379	0.009607	1	0.6967	0.99847	0.89839
2	0	12.109	0.018616	1	0.34182	0.99705	0.77962
3	0	0.018485	0.009021	1	0.99707	0.99857	0.99855
4	0	3.6889	0.000984	1	0.63029	0.99984	0.87671
5	0	7.1086	0.028924	1	0.46941	0.99542	0.82161
6	0	9.6895	0.015281	1	0.39359	0.99758	0.79705
7	0	5.376	0.002829	1	0.53913	0.99955	0.84623
8	0	9.9302	0.02781	1	0.38775	0.9956	0.79445
9	0	12.578	0.02002	1	0.33333	0.99683	0.77672
10	0	0.10805	0.006573	1	0.98311	0.99896	0.99402
11	0	4.74	0.03452	1	0.57022	0.99454	0.85492
12	0	2.1407	0.023228	1	0.74605	0.99632	0.91412
13	0	0.056122	0.020128	1	0.99116	0.99681	0.99599
14	0	0.50854	0.000361	1	0.92519	0.99994	0.97504
15	0	4.5213	0.021457	1	0.58176	0.9966	0.85945
16	0	1.131	0.013637	1	0.84757	0.99784	0.94847
17	0	7.329	0.013347	1	0.46181	0.99788	0.8199
18	0	8.24	0.012164	1	0.43286	0.99807	0.81031

Table 5. The response table for the mean grey relational grades

	A	B	C	D	E	F	G	H
Level 1	0.8433	0.9066	0.9266	0.8477	0.8637	0.8700	0.8891	0.8630
Level 2	0.9080	0.8876	0.8409	0.8613	0.8621	0.8687	0.8494	0.8588
Level 3		0.8327	0.8594	0.9179	0.9011	0.8882	0.8885	0.9051
Difference	0.0648	0.0739	0.0857	0.0702	0.0390	0.0195	0.0397	0.0463

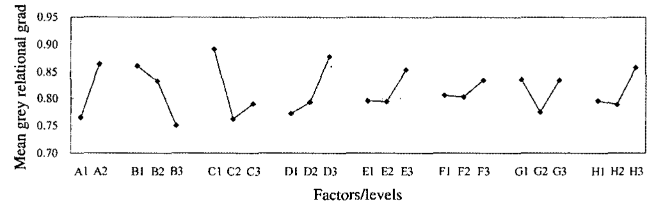

Figure 4. The response graph for the grey relational analysis.

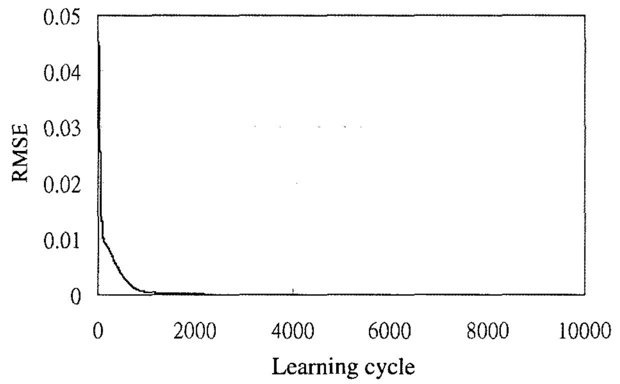

Figure 5. The RMSE diagram of the neural network.

< 59.4185, and $-6.5849 < \mu_{\text{twisting}} < -1.81052$. A total of five confirmation experiments were conducted for verification. From the optimum processing conditions of the single quality characteristic, the mean values of the hexagonal screw's outer diameter, tensile strength and twisting strength were 4.0218, 828.101, and 0.581, respectively, and their SN ratios were 46.141, 58.3617, and 4.7165, respectively. From the optimal processing conditions of the multiple quality characteristics, the mean values of the hexagonal screw's outer diameter, tensile strength and twisting strength were 4.0589, 843.967, and 0.6295, respectively, and their SN ratios were 53.8841, 58.5266, and -4.0201, respectively. Obviously, the SN ratios all fall within the 95 % confidence interval from the confirmation experiments. The results of the confirmation experiments indicated that the factor effects possessed reproducibility. It also meant that the results of the experiments were worth trusting. Furthermore, the molding quality of the hexagonal screws obtained from the optimum processing conditions for multiple quality characteristics exceeded those from the optimum processing conditions for the single quality characteristic.

Next, the PEEK quality prediction system shall be established using the results obtained from the previous Taguchi orthogonal

Table 6. The analysis of variance table for outer diameter/tensile strength/twisting strength

Source	Degree of freedom			Sum of square			Mean square			F test		
A	1	1	1	13.23*	0.10	0.01*	-	0.10	–	–	4.50	–
B	2	2	2	47.25	0.11	0.18*	23.62	0.05	–	2.72	2.49	–
C	2	2	2	190.71	0.12	0.92	95.36	0.06	0.46	10.99	2.68	2.61
D	2	2	2	65.10	0.01*	0.73	32.55	–	0.37	3.75	–	2.07
E	2	2	2	79.95	0.06*	0.28*	39.98	–	–	4.61	–	–
F	2	2	2	20.79*	0.06*	1.32	–	–	0.66	–	–	3.73
G	2	2	2	6.93*	0.04*	0.27*	–	–	–	–	–	–
H	2	2	2	24.60*	0.11	1.54	–	0.05	0.77	–	2.48	4.35
Error	2	2	2	12.61*	0.03*	0.85	–	–	–	–	–	–
(Pooled error)	(9)	(9)	(9)	(78.16)	(0.19)	(1.59)	(8.68)	(0.02)	(0.18)			
Total	17	17	17	436.02	0.62	6.09						

*The pool-up terms.

Table 7. The percentage errors for the target values and the predicted values

Test sets	Target value			Predicted value			Percentage error (%)		
	Diameter (mm)	Tensile strength (N)	Twisting strength (N·m)	Diameter (mm)	Tensile strength (N)	Twisting strength (N·m)			
1	3.994	828.1	0.508	4.032	820.99	0.516	0.9514	0.8586	1.5748
2	4.076	842.8	0.599	4.132	851.37	0.606	1.3739	1.0168	1.1686
3	4.06	823.2	0.511	4.0199	813.99	0.503	0.9877	1.1188	1.5656
4	4.017	828.1	0.537	4.063	820	0.541	1.1451	0.9781	0.7449
5	4.068	813.4	0.545	4.043	803.6	0.553	0.6146	1.2048	1.4679
6	4.062	808.5	0.549	4.088	813.6	0.557	0.6401	0.6308	1.4572

array experiment. Moreover, the differences between the predicted values and the target values were evaluated in order to achieve a precise prediction of the molding quality. The injection molding machine's eight control factors were input into BPNN as the input variables, and the values of the hexagonal screw's outer diameter, tensile strength and twisting strength were used as the output variables.

The experimental results of the Taguchi experiments would be as the training sets and the test sets. The twelve experiments of the L_{18} orthogonal array were used as training sets, and the other six experiments of the L_{18} orthogonal array were used as test sets. The learning rate and the momentum factor directly affected the convergence speed of the network, and the number of hidden neurons affected the complexity of the network. Hence, the training sets were used to obtain the optimum learning parameters first. The range set for the learning rate and momentum factor usually fall between 0 and 1, and 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, and 0.9 were adopted for the design. The two most common methods adopted for the number of hidden neurons were: (the number of input layers + the number of output layers)/2 and (the number of input layers + the number of output layer)$^{1/2}$, and 3, 4, 5, and 6 were adopted for the design. After 324 times of learning and comparing, the optimum convergence effect was discovered with the learning rate of 0.9, a momentum factor of 0.8, and the number of hidden neurons of 5. The RMSE of BPNN can converge to 0.00002 and the convergence curve is shown in Figure 5. When the network's training was completed, the test sets were applied to the network to find out if the neural network has a good prediction capability. The percentage errors between the target value and the predicted value were also calculated and are shown in Table 7. Because the maximum and minimum of the outer diameter were 4.1427 mm and 3.99 mm respectively, the target value was set at the average value 4.066 mm. From this, the absolute percentage error between target and maximum values as well as target and minimum values can be obtained. It is 1.5748 %. For this reason, the maximum deviation percentage of a prediction system is set to be 1.5748 %. The percentage errors obtained from Table 7 all fall within 1.5748 %, so this indicates that the control factors and their levels used for the prediction system are acceptable.

Conclusion

This study focused on the PEEK injection molding process using the Taguchi method and to make the experimental plan with the least number of experiments. However, the Taguchi method was used for obtaining the optimum processing combination for a single quality characteristic only, and did not give any consideration to the relationship between multiple quality characteristics and processing parameters. Therefore, the grey relational analysis was applied to improve the drawbacks of the Taguchi method and to achieve the purpose of optimization for multiple quality characteristics. As a result of the optimization of multiple quality characteristics, the dimensional deviation of the screw's outer diameter was successfully minimized, and the tensile strength and twisting strength were maximized in the meantime. In addition, a quality prediction system of the PEEK injection molding was also established. Through the learning network, the RMSE can converge to 0.00002. The predicted values and the target values of this prediction system are all within 1.5748 %, which also shows its accuracy. It also means that the control factors and their levels as well as the learning parameters of the neural network are well planned and effectively chosen. This also reveals the reproducibility and reliability of the experiment results. This study combines grey relational analysis with the Taguchi method for the optimization of the PEEK injection molding processing parameters. The efficiency of this optimization model had been successfully proven by experiments and can be compliant with the research purpose of taking active actions for waste prevention. Additionally, back-propagation neural network has advantage of multiple input and output variables; therefore, it does not be affected by the difference between the effects of control factors for the tensile strength and the twist strength as shown in Table 6. So the difference is acceptable for this prediction system. In the future, the optimization model will be further applied to the planning of other related processes as a point of reference for them.

References

1. W. H. Bonner, *U.S. Patent*, 3065205 (1962).
2. T. E. Attwood, P. C. Dawson, J. L. Freeman, L. R. J. Hoy, J. B. Rose, and P. A. Staniland, *Polymer*, **22**, 1096 (1981).
3. S. Sanchagrin, *Polym. Eng. Sci.*, **23**, 431 (1983).
4. A. Siegmann, A. Buchman, and S. Kenic, *Polym. Eng. Sci.*, **27**, 1069 (1987).
5. A. Siegmann, A. Buchman, and S. Kenic, *Polym. Eng. Sci.*, **22**, 560 (1982).
6. H. T. Pham, C. P. Bosnyak, and K. Sehanobish, *Polym. Eng. Sci.*, **33**, 1634 (1993).
7. K. M. Jansen, D. J. V. Dijk, and M. H. Husselman, *Polym. Eng. Sci.*, **38**, 838 (1998).
8. D. S. Choi and Y. T. Im, *Composite Structures*, **47**, 655 (1999).
9. T. C. Chang and E. Faison III, *Polym. Eng. Sci.*, **41**, 703 (2001).
10. C. L. Lin, J. L. Lin, and J. T. Huang, *The Journal of Grey System*, **4**, 359 (2001).
11. B. F. Yousef, G. K. Knopf, E. V. Bordatchve, and S. K. Nikumb, *Int. J. Adv. Manuf. Technol.*, **22**, 41 (2003).
12. S. S. Madaeni and S. Koocheki, *Chem. Eng. J.*, **119**, 37 (2006).
13. P. J. Kelly, R. D. Arnell, M. D. Hudson, A. E. J. Wilson, and G. Jones, *Vacuum*, **61**, 61 (2001).

14. J. M. Liu, P. Y. Lu, and W. K. Weng, *Mater. Sci. Eng. B-Solid State Mater. Adv. Technol.*, **85**, 209 (2001).
15. C.-F. J. Kuo and T. L. Su, *Text. Res. J.*, **73**, 461 (2003).
16. X. Zhang, S. Zhang, and Z. He, *J. Cryst. Growth*, **264**, 409 (2004).
17. D. Guo, Y. Wang, C. Nan, L. Li, and J. Xia, *Sens. Actuator A-Phys.*, **102**, 93 (2002).
18. A. J. Greaves, *Dyes Pigment.*, **46**, 101 (2000).