Performance prediction of tobacco flavouring using response surface methodology and artificial neural network

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Abstract: This study was to predict the optimum condition for leaf flavouring in cigarette manufacturing. To this purpose, an integrated research was used by using response surface and artificial neural network. A series of tobacco flavouring experiment's factors were designed by Experimental Design software. The MATLAB software's Neural Network function was used to forecast the responses, and the optimal solution configuration was coming out from the Response Surface Analysis Method. In the optimum condition, moisture removal opening, roller speed and tobacco process flow, pressure and feed liquid gas ejector flow are 18.60%, 10.74 rpm, 5314.11 kg/h, 3.70 bar and 243.63 kg/h, uniformity of the evaluation index and the integrated research was used by using response surface and artificial neural network. A series of tobacco flavouring experiment's factors were designed by Experimental Design software. The MATLAB software's Neural Network function was used to forecast the responses, and the optimal solution configuration was coming out from the Response Surface Analysis Method. In the optimum condition, moisture removal opening, roller speed and tobacco process flow, pressure and feed liquid gas ejector flow are 18.60%, 10.74 rpm, 5314.11 kg/h, 3.70 bar and 243.63 kg/h, uniformity of the evaluation index and the utilization rate of material liquid distribution are 93.08% and 98.694%. With the corresponding experimental, results are consistent, under the condition of the error to less 7%, the test results show that through a few experimental data of predictive results of the neural network and response surface design has a certain practicability.

1 Introduction

Cigarette casing technology refers to the process of flavouring (a source of liquid) on tobacco leaves, which can help to develop tobacco products with acceptable sensory quality and smoke chemical composition. Flavouring helps to reduce tobacco leaf's flaws of decoration and reduce the flue gas irritating. It can be achieved to improve the toughness and combustibility of tobacco, but also can improve the ability of tobacco anticorrosion [1]. The effect of tobacco and leaf casing determines the quality of silk and the subsequent sensory evaluation and user's smoking feel. Currently, the effect of flavouring mainly through to the material chemical tests such as 1,2 propylene glycol, which content in tobacco leaves after flavoured, uniformity in the characterisation of 1,2-propylene glycol as marker's detection methods of characterisation of test material liquid content in tobacco leaves to represent the utilisation rate. This paper has prepared 48 predicted sets of test data by using neural network training and the optimum solution configuration by using the response surface analysis method. Finally, the optimal solution was verified through the production line and good results were obtained

2 Methodology

2.1 Test data designs

Using Box-Behnken method of Response Surface Methodology in experimental design software Design-Expert with 5 factors [2]. The influence of the opening of the moisture removal (10–50%), tobacco cylinder rotational speed (7–12 rpm), tobacco process flow (5000–7000 kg/h), pressure of gas ejector (1–4.5 bar), material liquid flow (170–250 kg/h), selected as independent variables, namely moisture removal (MR), cylinder rotational speed (CRS), tobacco process flow (TPF), gas ejector pressure (GEP), and material liquid flow (MLF). Two responses, uniformity and material liquid utilisation ratio, namely UM and UR, were described by polynomial models. With MR, CRS, TPF, GEP and MLF as the independent variables, the uniformity of flavouring, to design the experiments and the utilisation rate of material liquid as the dependent variable, the 46 group of dates were designed to meet the test data of 5 variables, as shown in Table 1.

2.2 Experimental data for training by using neural network

According to the experimental data of the 46 groups, the neural network training of MATLAB (MathWorks, USA) was used to meet the requirements. BP neural network is a multi-layer feedforward network trained by the error-inverse propagation algorithm. The learning rule is a gradient descent method which is continuously adjusting the weights and thresholds of the network through the reverse propagation, and to minimise the error sum of the network. The BP neural network model topology includes input layer, hidden layer and output layer [3]. The learning process of the backpropagation algorithm consists of two processes: forward propagation of information and reverse propagation of error.

Nine groups data for neural network training come from the project of analysis on the effect of tobacco flavouring, as shown in Table 2.

2.2.1 Uniformity training and predicting: To determine the row of the MR, CRS, TPF, GEP, MLF and responses of the nonlinear relationship, one needs to determine the appropriate network structure, with 5 layers neural network structure model [4].

Using BP Neural Network Toolbox of MATLAB, Neural Network Time Series Tool (ntstool) was analysed, and the input layer to hidden layer uses Sigmoid function, Tansig as transfer function, transfer function of the output layer neurons Purelin.

The training function parameters are set as follows: the number of iterations is 1000. Also the rate of learning in network training is 0.1, and the error performance desired value is 0.0004.

The simulation analysis of 9 groups of data in Table 2 was work out with the trained neural network. Mapminmax function of the input sample data using MATLAB normalisation process to eliminate the dimension influence, improve the network convergence, built with newff function neural networks, chose trainlm after much comparison function using Bayesian regularisation algorithm in network training. Using MATLAB neural network tool for training, the minimum mean square error (mse) is 1.3335. After the network training, 9 sets of test data were used to predict the training model, and the Postmmx function was used to reverse the normalisation process for simulation results, and a more accurate BP neural network model was obtained.
Table 1  Experimental variables designed

| MR, % | CRS, rpm | TPF, kg/h | GEP, bar | MLF, kg/h |
|-------|----------|-----------|----------|-----------|
| 25    | 10.75    | 5000      | 2.5      | 175.00    |
| 35    | 10.75    | 6000      | 2.5      | 175.00    |
| 25    | 13.00    | 6000      | 1.5      | 201.25    |
| 25    | 10.75    | 7000      | 3.5      | 201.25    |
| 25    | 10.75    | 6000      | 1.5      | 175.00    |
| 25    | 8.50     | 7000      | 2.5      | 201.25    |
| 35    | 8.50     | 6000      | 2.5      | 201.25    |
| 25    | 10.75    | 6000      | 1.5      | 227.50    |
| 25    | 10.75    | 6000      | 2.5      | 201.25    |
| 25    | 13.00    | 6000      | 3.5      | 201.25    |
| 15    | 10.75    | 6000      | 2.5      | 201.25    |
| 15    | 10.75    | 7000      | 2.5      | 201.25    |
| 25    | 8.50     | 7000      | 2.5      | 201.25    |
| 15    | 13.00    | 6000      | 2.5      | 227.50    |
| 15    | 10.75    | 6000      | 2.5      | 175.00    |
| 15    | 10.75    | 6000      | 3.5      | 201.25    |
| 25    | 10.75    | 6000      | 2.5      | 201.25    |
| 15    | 10.75    | 6000      | 2.5      | 201.25    |
| 15    | 8.50     | 7000      | 2.5      | 201.25    |
| 35    | 10.75    | 5000      | 2.5      | 201.25    |
| 25    | 10.75    | 6000      | 2.5      | 201.25    |
| 25    | 13.00    | 7000      | 2.5      | 175.00    |
| 15    | 10.75    | 6000      | 2.5      | 201.25    |
| 15    | 10.75    | 6000      | 2.5      | 201.25    |
| 25    | 8.50     | 7000      | 2.5      | 201.25    |
| 25    | 10.75    | 6000      | 2.5      | 201.25    |
| 25    | 10.75    | 6000      | 2.5      | 201.25    |
| 35    | 8.50     | 6000      | 2.5      | 201.25    |

Table 2  Experimental original data

| MR, % | CRS, rpm | TPF, kg/h | GEP, bar | MLF, kg/h | UM, % | UR, % |
|-------|----------|-----------|----------|-----------|-------|-------|
| X1    | X2       | X3        | X4       | X5        | Y1    | Y2    |
| 15    | 13       | 5500      | 2.5      | 192.5     | 78.75 | 69.002|
| 25    | 8.5      | 5000      | 3.5      | 175.0     | 82.05 | 62.405|
| 35    | 10       | 6500      | 3.0      | 227.5     | 77.41 | 75.184|
| 30    | 11.5     | 6000      | 1.5      | 210.0     | 80.18 | 69.708|
| 20    | 7        | 7000      | 2.0      | 245.0     | 84.71 | 88.330|
| 30    | 10       | 7000      | 3.5      | 175.0     | 79.16 | 94.012|
| 15    | 7        | 7000      | 1.5      | 210.0     | 83.10 | 82.572|
| 20    | 8        | 6500      | 2.5      | 227.5     | 85.62 | 78.217|
| 20    | 9        | 6500      | 2.5      | 227.5     | 85.65 | 81.618|

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Through the neural network completed by training, 46 groups of input designed by the experiment were input, and the corresponding results of uniformity were obtained, as shown in Table 3.

2.2.2 Liquid utilisation training and predicting: In order to determine the five input variables and the utilisation ratio of liquid non-linear relations, we need to determine the appropriate network structure with 6 layer neural network modelling. The layer of input in BP neural network to the hidden layer adopts the Sigmoid function hyperbolic tangent Tansig as the transfer function, and the output layer neuron transfer function adopts the function Purelin. The training function parameters are set as follows: the number of iterations is 1000. Also the rate of learning in network training is 0.1, and the error performance desired value is 0.0004.

The simulation analysis of 9 groups of data in Table 2 was work out with the trained neural network. Mapminmax function of the input sample data using MATLAB normalisation processing to eliminate the dimension influence, improve the network convergence, built with newff function neural networks, choose trainlm after much comparison function using Bayesian regularisation algorithms in network training. Using MATLAB neural network tool for training. Through the neural network completed by training, 46 groups of input designed by the experiment were input, and the corresponding results of utilisation rate were obtained, as shown in Table 3.

2.3 Response surface method

The response surface method (RSM) is a statistical method to solve the problem of multivariate by using the reasonable design of

| MR, % | CRS, rpm | TPF, kg/h | GEP, bar | MLF, kg/h | UM, % | UR, % |
|-------|----------|-----------|----------|-----------|-------|-------|
| 25    | 10.75    | 5000      | 2.5      | 175       | 73.56 | 52.27 |
| 35    | 10.75    | 6000      | 2.5      | 175       | 78.94 | 64.05 |
| 25    | 13       | 6000      | 1.5      | 201.25    | 81.87 | 64.68 |
| 25    | 10.75    | 7000      | 3.5      | 201.25    | 87.15 | 82.33 |
| 25    | 10.75    | 6000      | 1.5      | 175       | 81.16 | 55.74 |
| 25    | 10.75    | 6000      | 2.5      | 201.25    | 82.43 | 68.53 |
| 25    | 8.5      | 7000      | 2.5      | 201.25    | 84.09 | 83.55 |
| 25    | 10.75    | 6000      | 2.5      | 201.25    | 82.43 | 68.53 |
| 35    | 8.5      | 6000      | 2.5      | 201.25    | 83.08 | 69.76 |
| 25    | 10.75    | 6000      | 1.5      | 227.5     | 84.34 | 76.22 |
| 25    | 10.75    | 6000      | 2.5      | 201.25    | 82.43 | 68.53 |
| 25    | 13       | 6000      | 3.5      | 201.25    | 75.42 | 82.93 |
| 25    | 8.5      | 6000      | 1.5      | 201.25    | 82.09 | 65.13 |
| 15    | 10.75    | 5000      | 2.5      | 201.25    | 76.61 | 48.33 |
| 15    | 10.75    | 7000      | 2.5      | 201.25    | 83.23 | 82.83 |
| 25    | 10.75    | 6000      | 2.5      | 201.25    | 82.43 | 68.53 |
| 35    | 10.75    | 5000      | 2.5      | 201.25    | 74.19 | 56.03 |
| 35    | 10.75    | 6000      | 2.5      | 227.5     | 75.03 | 74.52 |
| 15    | 13       | 6000      | 2.5      | 201.25    | 82.06 | 78.21 |
| 15    | 10.75    | 6000      | 3.5      | 175       | 84.11 | 79.73 |
| 15    | 10.75    | 6000      | 3.5      | 201.25    | 82.00 | 81.32 |
| 15    | 10.75    | 6000      | 2.5      | 227.5     | 83.94 | 73.60 |
| 25    | 10.75    | 6000      | 2.5      | 201.25    | 82.43 | 68.53 |
| 25    | 13       | 5000      | 2.5      | 201.25    | 68.06 | 63.11 |
| 25    | 10.75    | 6000      | 3.5      | 227.5     | 77.60 | 75.34 |
| 25    | 13       | 7000      | 2.5      | 201.25    | 86.61 | 80.84 |
| 25    | 13       | 6000      | 2.5      | 175       | 80.40 | 75.83 |
| 25    | 8.5      | 6000      | 2.5      | 227.5     | 86.08 | 77.58 |
| 15    | 10.75    | 6000      | 2.5      | 175       | 79.14 | 65.36 |
| 25    | 8.5      | 5000      | 2.5      | 201.25    | 77.87 | 49.92 |
| 35    | 10.75    | 6000      | 3.5      | 201.25    | 77.57 | 74.36 |
| 25    | 10.75    | 7000      | 2.5      | 175       | 83.65 | 83.08 |
| 25    | 10.75    | 5000      | 3.5      | 201.25    | 72.19 | 68.99 |
| 25    | 10.75    | 7000      | 2.5      | 227.5     | 85.81 | 79.01 |
| 25    | 13       | 6000      | 2.5      | 227.5     | 76.52 | 72.56 |
| 25    | 8.5      | 6000      | 2.5      | 175       | 84.99 | 55.21 |
| 15    | 10.75    | 6000      | 1.5      | 201.25    | 78.36 | 58.18 |
| 25    | 10.75    | 5000      | 1.5      | 201.25    | 73.05 | 46.84 |
| 25    | 10.75    | 6000      | 2.5      | 201.25    | 82.43 | 68.53 |
| 15    | 8.5      | 6000      | 2.5      | 201.25    | 80.28 | 64.76 |
| 35    | 10.75    | 7000      | 2.5      | 201.25    | 83.02 | 79.56 |
| 25    | 8.5      | 6000      | 3.5      | 201.25    | 88.29 | 73.38 |
| 25    | 10.75    | 7000      | 1.5      | 201.25    | 82.56 | 83.30 |
| 35    | 13       | 6000      | 2.5      | 201.25    | 73.33 | 72.89 |
| 25    | 10.75    | 5000      | 2.5      | 227.5     | 70.48 | 64.24 |
| 35    | 10.75    | 6000      | 1.5      | 201.25    | 78.03 | 66.87 |
experiment. To find the optimal process parameters the method was used by fitting function relation between factors and response value and analyzing regression equation. According to the prediction data of Table 3, data optimisation and optimal configuration are carried out by experimental design software ‘Design-Expert’, trial version 11, box-behnken test Design method [2]. The input variable is five factors, respectively, MR, CRS, TPF, GEP, MLF, and the output variable are two, respectively, for the UM and UR.

Analysis of variance (ANOVA) was applied to evaluate their statistical significance. In the ANOVA, the significance of the constant term, one-time item, quadratic term (interaction phase) and square (surface active) of the quadratic differential model is tested. Click on the optimisation button in the design-expert software, then click numerical, and select the maximum response value (maximum) in the range of test factors, and the combination is optimised for the following sets of data, among which the first group is the optimal combination.

2.4 Flavouring performance detection

2.4.1 Uniformity detection method: The addictive property of tobacco leaf is usually measured by the addictive of 1,2 propylene glycol in space [5]. The homogeneity of the addictive was characterised by the uniformity of 1,2 propylene glycol content on the tobacco leaves. The calculation formula of the uniformity coefficient CU% is

\[
CU\% = 100 - RSD\% = 100 - \frac{SD}{\bar{X}} \times 100
\]

(1)

where CU is the charging uniformity coefficient, RSD is the relative standard deviation, SD is the standard deviation, \(\bar{X}\) is the arithmetic average, \(X_i\) is an index value, and \(n\) is the number of an index value

2.4.2 Test method for material utilisation ratio: The test method of 1,2-propanediol as the marker was used to characterise the content of the liquid in the test tobacco leaves, and the expression of the equation of the uniformity and utilisation can be obtained as

\[
Q = \frac{q_l}{q_e} \times W \times 100\%
\]

(2)

Among them, \(q_l\) is the content of 1,2-propanediol in tobacco leaves of the unit quality, mg/g; \(q_e\) is the weight of 1,2-propanediol in the brand liquid, mg/g. \(W\) is the proportion of the brand feeding, %.

3 Results

3.1 Artificial neural network (ANN) results

Six ANN architectures were tested for input parameters, varying the number of hidden layers, epoch’s number and momentum [6]. Through the neural network completed by training, 46 groups of input designed by the experiment were input, and the corresponding results of uniformity were obtained as shown in Table 3.

3.2 RSM results

RSM was applied to optimise the responses considering nonlinear, quadratic and interaction effects among independent variables. Fig. 1a shows the results of only two responses (MR and DRS). After the interaction between various factors, the quadratic equation of the uniformity and utilisation can be obtained as

\[
\begin{align*}
UM & = 7.0319 + 0.142x_1 + 0.677x_2 + 1.623 \times 10^{-3}x_1^3 \\
& \quad - 9.800x_1 + 0.109x_1 + 0.130x_2 - 2.153 \times 10^{-3}x_1x_2 \\
& \quad - 0.277x_3 - 1.534 \times 10^{-3}x_3x_4 - 3.864 \times 10^{-3}x_5 \\
& \quad - 0.776x_1 - 0.015x_3 + 2.287 \times 10^{-3}x_4 \\
& \quad - 5.382 \times 10^{-3}x_5 + 0.047x_5 + 7.128 \times 10^{-3}x_7^2 \\
& \quad + 0.135x_1 + 1.005 \times 10^{-3}x_2^2 + 1.128x_3^2 + 8.326 \times 10^{-3}x_4^2 \\
\end{align*}
\]

(3)

\[
\begin{align*}
UR & = 60.722 - 5.21x_1 + 35.733x_2 + 0.046x_3 + 0.046x_4 \\
& \quad + 29.047x_5 + 0.510x_6 - 7.509 \times 10^{-3}x_7 + 3.398 \\
& \quad \times 10^{-3}x_1x_2 + 0.251x_1x_3 + 3.204 \times 10^{-3}x_2x_3 \\
& \quad - 0.237x_3x_4 + 0.14858x_5 - 9.525 \times 10^{-3}x_5x_6 \\
& \quad - 2.288 \times 10^{-3}x_7 - 0.087x_7 + 0.013x_7^2 - 0.718x_8^2 \\
& \quad - 2.598 \times 10^{-3}x_9^2 + 0.344x_2 - 1.009 \times 10^{-3}x_7^2 \\
\end{align*}
\]

(4)

Contour plots of MR, CRS, TPF, GEP, MLF, UM and UR RSM models are depicted in Figs. 1 and 2. About the values of MR (20–40%) and CRS (7–2 rpm), UM increased, in the middle, near of MR30%, and raising by CRS. The optimal condition of tobacco feeding was determined by using the optimal solution function of RSM of the Design Expert software. The result in Table 4 shows that the optimised condition

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was the opening of the moisture removal 18.6%, drum rotational speed 10.74 rpm, tobacco process flow 5314 kg/h, pressure of gas ejector 3.7 bar and material liquid flow 243 kg/h, with the reasonable response is uniformity 93.09% and material liquid utilisation ratio 88.69%.

### 3.3 Comparison of consequences

According to the three optimal solutions, corresponding tests were carried out in the production line. The uniformity and utilisation rate were calculated by measuring the content of 1,2 propanediol in tobacco leaves. The results of detection and RSM are shown in Fig. 3.

According to the test and prediction results, the general trend of aromatherapy effect is consistent, and the optimal solution is also corresponding. The maximum relative error is controlled within 7%, which has a good reference value. Also the best conditions are obtained.

### 4 Conclusion

Based on neural network training of MATLAB, the data of the training and experimental design were predicted, and the optimal

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**Table 4** Optimisation with RSM

| MR, % | CRS, rpm | TPF, kg/h | GEP, bar | MLF, kg/h | UM, %  | UR, %  |
|-------|----------|-----------|----------|-----------|--------|--------|
| 16.1  | 8.78     | 5259      | 3.7      | 199       | 92.64  | 88.57  |
| 15.4  | 10.29    | 5930      | 3.7      | 222       | 93.85  | 87.18  |
| 18.6  | 10.74    | 5314      | 3.7      | 243       | 93.09  | 88.69  |
solution was obtained through the response surface analysis, and the intelligent prediction of the process of tobacco processing was realised. The results show that the neural network model can achieve the accuracy of 7% by neural network training. The basic data of experimental design is the premise of obtaining high precision and optimal solution. Throughout the optimal solution, moisture removal opening is 18.60%, tobacco cylinder rotational speed is 10.74 rpm and tobacco process flow of 5314.11 kg/h, gas ejector pressure is 3.7 bar, material flow rate is 243.63 kg/h, under the condition of tobacco feeding evaluation index evenness is 93.088, the utilisation ratio is 88.694. Under reasonable input configuration, it can greatly improve the absorption of tobacco leaves, significantly improve the casing performance of tobacco leaf, this shows that the neural network and response surface intelligent prediction can be achieved under the action of certain guiding significance.

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