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Optimizing brake cup formulation using mixture experiments and principal component regression model

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This study focuses on developing an optimal formulation to improve reliability of brake cup for motors. Designs mixtures experiments were performed based on quadratic models. Principal component regression was then utilized to resolve collinearity problem among designed ingredients to establish response surface model for each physical property. Multiple physical properties of brake cup were simultaneously considered to determine optimal formulation using desirability function to enhance reliability. A real case demonstrates effectiveness of successfully developed high reliability brake cup at low manufacturing cost.

Keywords: Brake cup, Mixture experiment, Optimization, Principal component analysis

Introduction

Brake cup is an important rubber compound component of brake system for motors. Formulation of rubber material involves selecting various types of ingredients and determining their optimal formulation to obtain high product reliability[1]. After meeting required specifications of physical properties of rubber materials, a dynamic test is conducted for determining reliability using computer-aided design algorithms[2,3] (A-, D-, G-, and V-optimality). Dabbas *et al*[4] resolved complex scheduling problem for a semiconductor manufacturing system using experiments with mixture and desirability function[5]. Brandvik *et al*[6] optimized oil dispersant composition using experiments with mixtures and response surface model. Correia[7] explored linear firing shrinkage and water absorption of triaxial ceramic bodies using experiments with mixtures.

This study presents development of an optimal formulation to optimize physical properties of rubber compound components. Principal component analysis (PCA) was employed to resolve collinearity among designed ingredients. PCA was conducted on designed ingredients' points to obtain several independent components. Then, response surface model with respect to each physical property of brake cup was fitted on these components. Finally, multiple properties of brake cup were simultaneously considered on the basis of fitted models to determine optimal formulation using desirability function to enhance product reliability.

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Experimental

Experiments with Mixtures

When experimental factors (ingredients) and response values are function of proportion, rather than absolute amount, process of solution is called experiments with mixtures. Designed experimental points are determined on the basis of ingredient proportion. Each proportion falls in an interval of zero and one. As summation of all ingredient proportion is equal to one, degree of feasible ingredients region reduces to one dimension. Space of feasible solution is a constrained experimental region. Ingredients proportions are regarded as independent variables to fit a response surface model[8] in mixture experiments as

$$\eta = \sum_{i=1}^{q} \beta_i^* x_i + \sum_{i \le j}^{q} \sum_{j}^{q} \beta_{ij}^* x_i x_j + \sum_{i \le j \le k}^{q} \sum_{j \le k}^{q} \sum_{k}^{q} \beta_{ijk}^* x_i x_j x_k + \cdots \quad \ldots(1)$$

where $\beta_i^* = \beta_0 + \beta_i + \beta_{ii}$, and $\beta_{ij}^* = \beta_{ij} - \beta_{ii} - \beta_{jj}$. From Eq (1), source of curve response variation is mixture effects among various types of ingredients, exhibiting in a high-order term.

Principal Component Analysis (PCA)

PCA is used to resolve collinearity problem in establishing regression model, due to existence of high correlation among independent variables. PCA is applied on independent variables to obtain several uncorrelated components, which are linear combination of original independent variables[9,10] as

$$\begin{aligned} \xi_1 &= w_{11}x_1 + w_{12}x_2 + \cdots + w_{1p}x_p \\ \xi_2 &= w_{21}x_1 + w_{22}x_2 + \cdots + w_{2p}x_p \\ &\vdots \\ \xi_p &= w_{p1}x_1 + w_{p2}x_2 + \cdots + w_{pp}x_p \\ i, j &= 1, 2, \cdots, p \end{aligned} \quad \ldots(2)$$

where, ξ_i represents principal component score of i^{th} component; $i = 1,\ldots, p$; w_{ij} denotes a weight of j^{th} variable of i^{th} component. Composed of weights are referred as Eigenvector. All weighs conform constraints of $w_{i1}^2 + w_{i2}^2 + \cdots + w_{ip}^2 = 1$, and $w_{i1}w_{j1} + w_{i2}w_{j2} + \cdots + w_{ip}w_{jp} = 0$, $i \ne j$

Variances of principal components are referred as Eigenvalues. Sum of variances of principal components is equal to sum of variances of original variables. A thumb rule in PCA is that retaining component with its Eigenvalue is greater than 1. Retained uncorrected components, which are then treated as independent variables, fit a regression model on response variables. If a second-order model is appropriate, this model can be expressed as

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i \xi_i + \sum_{i=1}^{k} \beta_{ii} \xi_i^2 + \cdots + \sum \sum_{i<j} \beta_{ij} \xi_i \xi_j + \varepsilon \quad \ldots(3)$$

where, y represents response variable, ξ_i denotes a linear effect of i^{th} component, $i = 1,\ldots,k$ ξ_i^2 indicates a quadratic effect of i^{th} component, $\xi_i \xi_j$ is an interaction effect between i^{th} component and j^{th} components, and ε is a random error term.

Variance inflation factor (VIF) evaluates degree of collinearity in establishing regression model[11] as

$$VIF_i = 1 \big/ \left(1 - R_i^2\right), \quad i = 1, 2, \cdots, p-1 \quad \ldots(4)$$

where VIF_i represents *VIF* value of i^{th} independent variable, R_i^2 is a determinant coefficient of regression model of i^{th} variable on e other $p-2$ variables. A large *VIF* value indicates a serious collinearity problem. Generally, criteria of VIF≥10 exhibits high degree of collineartiy among independent variables, decreasing model robustness because of high variance of predicted value.

Proposed Procedure

Proposed procedure for optimal formulation for brake cup components has six steps (Fig. 1).

Step 1: Design Experiments with Mixtures

Simplex lattice design is employed to design experiment in case of formulation of simplex experimental region. D-optimality algorithm is employed to design experiment when experimental region is no longer a simplex region.

Step 2: Test Degree of Collinearity among Designed Ingredients

Index value of *VIF* is calculated using Eq. (4) to evaluate degree of collinearity. If value of *VIF*≥10, this result indicates a high correlation exists among designed ingredients, causing a collinearity problem in fitting response surface model on these designed ingredients.

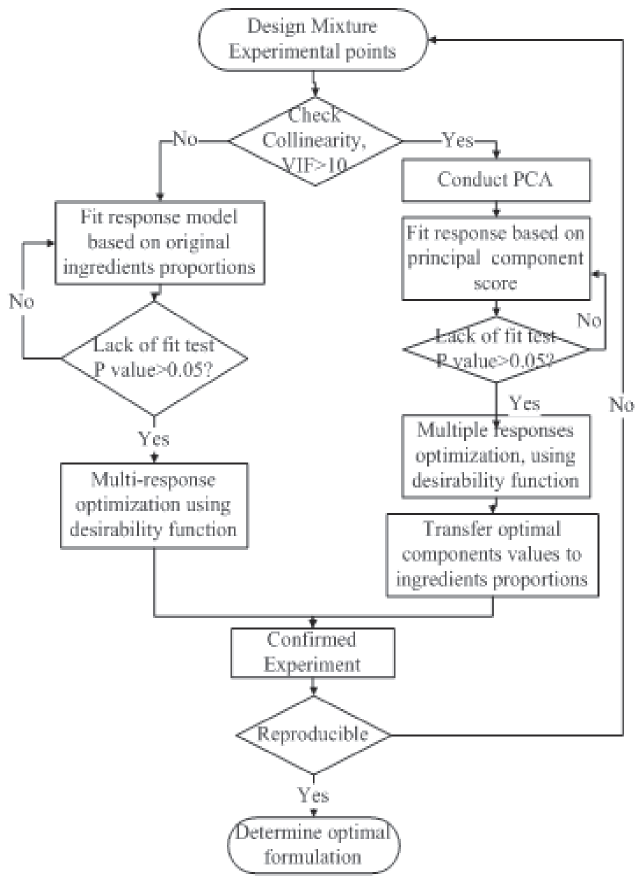

Fig. 1—Proposed optimization process

In this regard, PCA technique is used to establish response surface model. If value of *VIF* is not greater than 10, no collinearity problem is concerned, and general regression technique is used to establish response surface model.

Step 3: Conduct PCA on Designed Ingredients

PCA is initially conducted on designed ingredients to obtain several independent components having their eigenvalues greater than 1. Response surface models are then fitted on these components using Eq. (3).

Step 4: Conduct Lack of Fit Test

Lack of fit test is utilized to determine an appropriate response surface model. If P value of lack of fit test is greater than 0.05, no sufficient evidence indicates inappropriateness of model at significance level $\alpha = 0.05$. Accordingly, an appropriate response model can be obtained.

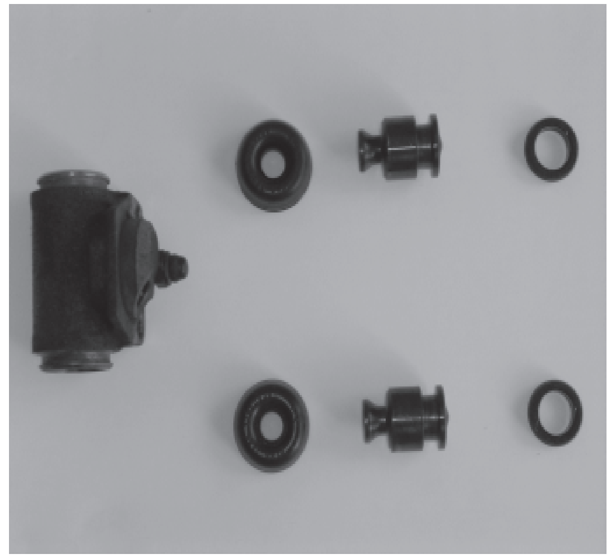

Fig. 2—Components of brake cup

Step 5: Determine Optimal Value of Independent Component

This study used statistical experiment software, Design Expert, to establish response surface models. Optimal values of independent components were determined using desirability function[5], embedded in Design Expert software, to resolve multi-response optimization problem. Subsequently, substituting optimal values of independent components into Eq. (2), and considering constraint that summation of all ingredients proportions is 1, optimal ingredients proportions can be obtained. If general regression model is used to establish response surface model, optimal ingredients proportions can be directly obtained.

Step 6: Conduct Confirmed Experiments

Confirmed experiments were conducted under optimal ingredients proportions obtained from Step 5 to verify reproducibility of optimal condition. If optimal condition cannot be reproduced, suitable ingredients and their lower and upper constraints must be determined prior returning to Step 1.

Case Study

Brake cup is an essential oil seal [ingredients: rubber, 83.3%; (anti-oxidant, flow admixture A, flow admixture B and crosslinking agents), 16.7%], which functions primarily to prevent oil leakage (Fig. 2). Of four designed ingredients, lower and upper constraints, respectively, are as follows: anti-oxidant, 1.00, 2.80; flow admixture A, 2.20, 4.20; flow admixture B, 2.20, 4.20; and crosslinking agents, 5.56, 11.15 %. Thus, designed feasible region is no longer a simplex region. D-optimality algorithm was used to design experiments based on a quadratic model. Given the resource of conducting experiments, 15 runs (designed points, 10; replicate points, 3; and check points, 2) were performed. Physical properties [hardness (H), elongation (E), and tensile strength (TS)] were recorded. Response value of H is desired target (60), but cannot be greater than 75. Response values of E and TS are largely desired and have lower specification limit as follows: E, 200%; and TS, 100 kgf/cm^2. According to proposed optimal procedure of brake cup, these three response values were analyzed. VIF values of four designed ingredients are as follows: anti-oxidant, 4.2; flow admixture A, 5.6; flow admixture B, 6.7; and crosslinking agents, 12.5. VIF value of crosslinking agents (>10) exhibits a collinearity problem among designed ingredients points in establishing response surface model. This is because severe lower and upper constraints are set for each ingredient, shrinking feasible region, and causing high correlation among designed experiment points.

Table 1—Eigenvalues of each independent component

	Eigenvalues	Total variance %	Cumulative %
Component A	1.906495	47.66238	47.6624
Component B	1.161240	29.03101	76.6934
Component C	0.932264	23.30659	100.0000

Table 2—Eigenvector of each independent component

Eigenvector	Component A	Component B	Component C
Anti-oxidant	-0.486435	-0.049332	0.765334
Flow admixture A	-0.339555	0.736681	-0.401097
Flow admixture B	-0.356464	-0.674153	-0.496684
Crosslinking agents	0.721815	-0.019623	0.081795

Therefore, PCA technique was utilized to establish response surface model.

For three components (Component A, Component B and Component C), eigenvalues (Table 1) and eigenvectors (Table 2) of each component were listed. These three components were retained to fit response surface models with respect to H, E and TS. P value of model is 0.0001. P value for lack of fit test of linear model for H is 0.8806, which is insignificant at significance level 0.05, indicating fitted linear model is appropriate. Besides component B, components A and C significantly affect to H (Table 3) as

$$H = 62.67 + 1.89 \times \textit{component}\ \mathrm{A} + 0.43 \times \textit{component}\ \mathrm{B} - 1.57 \times \textit{component}\ \mathrm{C},\ R^2 = 0.8611$$

P value for lack of fit test of quadratic model for E is 0.57, which is insignificant at significance level 0.05, indicating fitted quadratic model is appropriate. Component A affects to E significantly (Table 4) as

$$\mathrm{E} = 184.46 - 51.79 \times \textit{component}\ \mathrm{A} - 3.89 \times \textit{component}\ \mathrm{B} + 23.49 \times \textit{component}\ \mathrm{C} + 8.63 \times (\textit{component}\ \mathrm{A})^2 - 8.97 \times (\textit{component}\ \mathrm{B})^2 + 3.65 \times (\textit{component}\ \mathrm{C})^2 + 3.53 \times \textit{component}\ \mathrm{A} \times \textit{component}\ \mathrm{B} - 18.65 \times \textit{component}\ \mathrm{A} \times \textit{component}\ \mathrm{C} - 6.09 \times \textit{component}\ \mathrm{B} \times \pm\ \textit{component}\ \mathrm{C},\ R^2 = 0.99$$

P value for lack of fit test of linear model for TS is 0.8941, which is insignificant at significance level 0.05, indicating fitted linear model is appropriate. Components A and C significantly affect TS but not component B (Table 5) as

$$\mathrm{TS} = 134.53 - 13.56 \times \textit{component}\ \mathrm{A} + 2.03 \times \textit{component}\ \mathrm{B} + 14.69 \times \textit{component}\ \mathrm{C},\ R^2 = 0.8795$$

Table 3—ANOVA on hardness

Variation source	SS	df	MS	F	P value
Model	130.31	3	43.44	22.73	0.0001
Component A	94 .92	1	94.92	49.66	0.0001
Component B	3.02	1	3.02	1.58	0.2346
Component C	32.36	1	32.36	16.93	0.0017
Residual	21.02	11	1.91		
Lack of fit	10.52	8	1.32	0.38	0.8806
Pure error	10.50	3	3.50		
Total	151.33	14			

Table 4—ANOVA on elongation

Variation source	SS	df	MS	F	P value
Model	80012.39	9	8890.27	83.09	0.0001
Component A	60266.40	1	60266.40	427.70	0.0001
Component B	209.27	1	209.27	1.49	0.2773
Component C	4668.38	1	4668.38	33.13	0.0022
A^2	1717.03	1	1717.03	12.19	0.0175
B^2	420.62	1	420.62	2.99	0.1446
C^2	54.23	1	54.23	0.38	0.5622
AB	77.57	1	77.57	0.55	0.4915
AC	650.58	1	650.58	4.62	0.0844
BC	162.01	1	162.01	1.15	0.3326
Residual	704.54	5	140.91		
Lack of fit	682.04	2	341.02	45.47	0.0057
Pure error	22.50	3	7.50		
Total	80716.93	14			

Table 5—ANOVA on tensile strength

Variation source	SS	df	MS	F	P value
Model	7793.85	3	2597.95	26.76	0.0001
Component A	4909.16	1	4909.16	50.57	0.0001
Component B	67.09	1	67.09	0.69	0.4235
Component C	2817.61	1	2817.61	29.02	0.0002
Residual	1087.88	11	97.08		
Lack of fit	517.38	8	64.67	0.35	0.8941
Pure error	550.50	3	183.50		
Total	8861.73	14			

Desirability function embedded in Design Expert software gave optimal components values as follows: component A, -1; component B, 0.85; and component C, 0.09. Optimal H, E and TS values were found to be 61.0123 (component A), 253.314 (component B) and 151.068 (component C). Accordingly, optimal values of original ingredients proportions can be calculated using step 5 of proposed procedure. Optimal formulation of four ingredients was found as: anti-oxidant, 0.024; flow admixture A, 0.04; flow admixture B, 0.028; and crosslinking agents, 0.075. Confirmed experiments under optimal formulation were conducted and response values were found as: H, 60; E, 275; and TS, 157. Thus response values for H, E and TS meet specification requirement. Therefore, subsequent dynamic test was conducted to determine brake cup reliability. Product reliability was evaluated using dynamic test rig.

Conclusions

Given severe constraints of each mixture ingredient, D-optimality algorithm was used to design experiments. PCA technique was used to resolve collinearity problem and efficiently establish a robust response surface model for reducing cost and time in new product/process development. A real case demonstrated effectiveness of proposed optimization procedure. Although proposed procedure is primarily on brake cup component, it can be extensively used in any component development involving mixture experiments. Therefore, developed procedure both has generality and practicability.

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