Int J Adv Manuf Technol (2008) 35:769–777
DOI 10.1007/s00170-006-0754-5

ORIGINAL ARTICLE

The use of mixture experiments in tolerance allocation problems

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Received: 14 July 2005 / Accepted: 2 August 2006 / Published online: 20 December 2006

Abstract The response surface methodology (RSM) approach can be used to determine the optimal component tolerances in an assembly. Frequently, response surface designs such as Box-Behnken design and central composite design are used in tolerance allocation problems. In this article, mixture experiments, which are essentially constructed for designing a blend composition, are proposed instead of response surface designs in order to observe the cost values. Also some advantages and disadvantages of mixture designs are discussed.

Keywords Tolerance allocation · Response surface methodology · Mixture experiments

1 Introduction

Some products are composed of parts or components manufactured on different processes. In practice, tolerances of assembled products are specified according to functional requirements and tolerances of individual components. One of the most widespread methods for selecting the optimum tolerances is to formulate the tolerance allocation problem as a nonlinear optimization problem, using some manufacturing cost-tolerance functions to estimate a functional relationship between manufacturing cost and component tolerance. A summary of several cost-tolerance models is given in Kim and Cho [1]. In their study, they proposed a response surface design such as central composite or Box-Behnken design to estimate the manufacturing cost-tolerance function. In a similar paper, which was written by Jeang [2], a total cost function, which is the sum of manufacturing cost and quality loss, is proposed instead of manufacturing cost.

In this study, mixture designs, which are a special class of response surface designs are proposed to estimate cost-tolerance functions as an alternative to central composite and Box-Behnken designs. This study is organized as follows. First, a review of the response surface design model, which is previously proposed by Kim and Chou [1], is given. Mixture experiments, designs and their adaptation to tolerance allocation problems are discussed. Then, some possible advantages of mixture designs to CCD and BBD are discussed and an example using a mixture design is illustrated. In the last section, a brief conclusion is drawn.

2 Reviewing the studies about the use of response surface designs for tolerance allocation

Kim and Chou [1] formulate the tolerance allocation problem as minimize

$$\eta(t_1, t_2, \ldots, t_k)$$

subject to

$$t_1 + t_2 \ldots + t_k \leq T \quad (stack - up\ constraint)$$

$$l_i \leq t_i \leq u_i,\ i = 1, 2, \ldots, k \quad (design\ parameter\ constraint) \tag{1}$$

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where t_i is the tolerance of the ith component, T is stack- up tolerance, l_i and u_i are the lower and upper bounds of interest on t_i, respectively, and $\eta(t_1, t_2, ..., t_k)$ is the cost-tolerance function which its functional form is unknown.

In most industrial problems, the true functional form of the cost-tolerance relationship for each component is usually unknown. Therefore, Jeang [2] and Kim and Cho [1] propose response surface methodology (RSM) for analyzing the tolerance allocation problem statistically. RSM is a combination of statistical and mathematical techniques useful for modelling and analysis of the relationship between the response variable and several input (or design) variables. In RSM, the true and probably complex relationship between the response variable and input variable is approximated by a first or second order polynomial function. The comprehensive details for RSM can be found in [3, 4] and [5]. The predicted first order response function ŷ can be written as

$$\widehat{y} = \widehat{\beta}_0 + \sum_{i=1}^{k} \widehat{\beta}_i x_i \tag{2}$$

where $\widehat{\beta}_0$ and $\widehat{\beta}_i$ are estimated coefficients, which are found through the least squares method and x_is are the coded input variables. First order response surfaces designs, such as factorial or fractional factorial designs, can be used to obtain the estimated coefficients. Furthermore, the predicted second order response function can be written as

$$\widehat{y} = \widehat{\beta}_0 + \sum_{i=1}^{k} \widehat{\beta}_i x_i + \sum_{i \leq j} \sum \widehat{\beta}_{ij} x_i x_j \tag{3}$$

where $\widehat{\beta}_{ij}$ are estimated coefficients associated with second order (quadratic when $i=j$ and interaction when $i \neq j$) effects. Second order designs such as Box-Behnken or central composite designs can be used to obtain the estimated coefficients.

In Kim and Cho [1]'s study $\widehat{y}$ and x_is are regarded as manufacturing cost and coded form of component tolerances t_is, respectively where coding formula can be written as

$$x_i = \frac{2t_i - (u_i + l_i)}{u_i - l_i}, \quad i = 1, 2, ..., k. \tag{4}$$

When the true cost-tolerance function is approximated by a second order polynomial model, the tolerance allocation problem given in Eq. (1) can be rewritten as follows: Minimize

$$\widehat{y} = \widehat{\beta}_0 + \sum_{i=1}^{k} \widehat{\beta}_i x_i + \sum_{i \leq j} \sum \widehat{\beta}_{ij} x_i x_j$$

subject to:

$$\sum_{i=1}^{k} \frac{x_i(u_i - l_i) + (u_i + l_i)}{2} \leq T \quad (stack - up\ constraint)$$

$$-1 \leq x_i \leq 1\ , i = 1, 2, ..., k.\ (design\ parameter\ constarints) \tag{5}$$

In both Kim and Cho [1]'s and Jeang [2]'s studies, it is emphasized that the second order response surface designs such as Box-Behnken and central composite designs can be used to estimate the coefficients of a second order polynomial model. In the following sections, mixture designs, which are essentially used to obtain the best mixture (or formulation) where a product is composed by several ingredients, are proposed as an alternative to second order response surface designs and some advantages of mixture designs are discussed.

3 The use of mixture experiments for tolerance allocation

3.1 Review of mixture experiments

A mixture experiment is an experiment in which the response is a function of the proportions of the components present only in the mixture and is not a function of the total amount of the mixture. The general purpose of mixture experimentation is to make possible estimates, through a response surface exploration of the properties of an entire multi-component system from only a limited number of observations. Unlike the usual response surface problem where the concomitant variables represent quantitative amounts, in the mixture problem, the components represent proportions of a

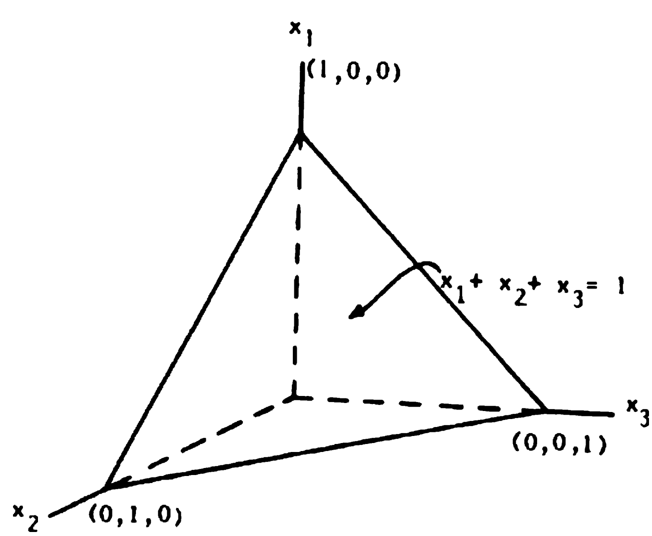

Fig. 1 Simplex factor space for $k = 3$

mixture or composition. These proportions must be nonnegative and if expressed as fractions of the mixture, they must sum to unity. For example, suppose there are k components in the system under study. If we represent the proportion of the ith component in the mixture by x_i, then

$$0 \leq x_i \leq 1, \tag{6a}$$

$$\sum_{i=1}^{k} x_i = 1 \tag{6b}$$

The factor space containing the k components may be geometrically represented by the interior and boundaries (vertices, edges, faces) of regular $(k-1)$ dimensional simplex. The vertices will represent mixtures consisting of single components and interior points will be the result of combining all the components. Figure 1 displays the factor space for k=3.

In general predicted linear and quadratic mixture models are: Linear:

$$\hat{y} = \sum_{i=1}^{k} b_i x_i \tag{7}$$

Quadratic:

$$\hat{y} = \sum_{i=1}^{k} b_i x_i + \sum \sum_{i<j}^{k} b_{ij} x_i x_j \tag{8}$$

Because of the restriction $x_1 + x_2 + ... + x_k = 1$, quadratic terms $b_{ii} x_i^2$ and the constant term b_0 are removed from the standard polynomial models.

Scheffe [6] introduced simplex lattice designs for mixture experiments and developed polynomial models, which have exactly the same number of terms as there are points in the associated designs. The designs, consisting of a symmetrical arrangement of points, are referred to as $\{k, m\}$ lattices. Corresponding to the points in a $\{k, m\}$ lattice, the proportions used for each of the k components have the m+1 equally spaced values from 0 to 1, that is, x_i=0, 1/m, 2/m,...,1 and all possible mixtures with these proportions for each component are used. The number of points in a $\{k, m\}$ lattice is $\binom{m+k-1}{m}$ and the lattice designs are characterized by their simplicity of construction. The details about lattice designs can be found in [7].

Frequently, one is not completely free to explore the entire simplex because of certain additional restrictions (physical and economic) that are placed on some or all components lower and upper bounds,

$$0 \leq a_i \leq x_i \leq b_i \leq 1 \tag{9}$$

Constraints (6b) and (9) can produce either of two types of experimental regions. One type of region is a result of the special situation where all of components are bounded above or all the components are bounded below or, in some instances, the components are all bounded above and below and have equal ranges. The resulting space has k vertices and is a simplex in terms of pseudo components. For this case, the recommended design for the quadratic model is the pseudo component simplex design, recommended by Kurotori [8].

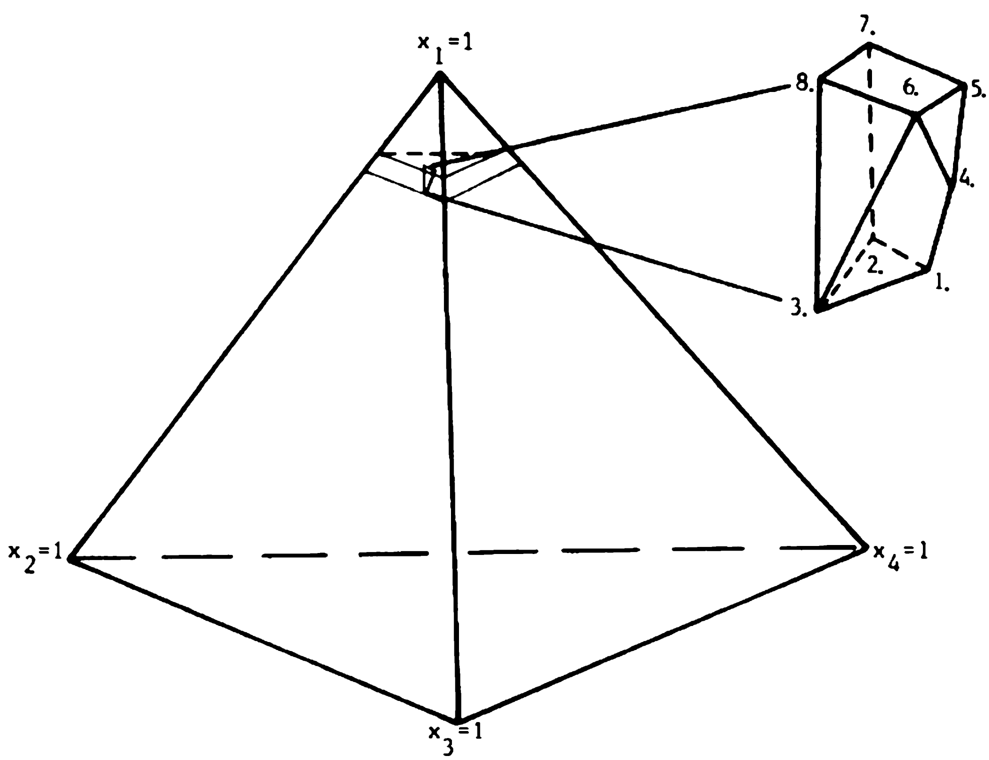

Fig. 2 An example of a constrained region

Table 1 The Number of design points of three different designs for second order model

Number of components	Mixture design	CCD	Box-Behnken design
3	6–9**	15	13
4	10***	25*	25
5	21	27*	41
6	48	45	49

*with half fractional factorial
**minimum number of design points is 4 and number of parameter is 6
*** minimum number of design points is 9 and number of parameter is 10
Source: R. A. McLean, and V. L. Anderson, (1966)

In most mixture problems, constraints (6) and (9) produce an irregular hyper polyhedron, which is a subspace of the k−1 dimensional simplex. An example of such a constrained region is drawn in Fig. 2. McLean and Anderson [9] recognized that the simplex designs were not generally applicable when both upper and lower limits were placed on the components and recommended the extreme vertices design. Crosier [10] presents a formula for calculation the number of vertices of any constrained region. When fitting the second order mixture model (8), generally support points consist of a subset of the extreme vertices of the region, edge centroids, or face centroids (if $k \geq 7$), and centroids of some of the r-dimensional flats (if $3 \leq k \leq 6$, then $2 \leq r \leq k-1$; and if $k \geq 7$, then $3 \leq r \leq k-1$). A centroid of an r-dimensional flat ($r \leq k-1$) is the average of all the vertices, which lie on the same constrained plane [7]. Snee and Marquardt [11], McLean and Anderson [9], Piepel [12], and Nigam et al. [13] discuss several algorithms that can be used to determine the coordinates of the extreme vertices of the constrained region and suggest formulas for calculating the number of vertices and higher dimensional boundaries of the region. Practically, these designs can easily be constructed in statistical packages such as SAS or MINITAB. SAS and MINITAB packages can select a subset of the extreme vertices and convex combinations of the vertices as design points, depending on D-optimality or A-optimality criteria of designs. Comprehensive details for mixture experiments are in [7].

3.2 Adaptation of mixture experiments to tolerance allocation problems

One advantage of using mixture experiments for tolerance allocation problems is that they require fewer runs than classical response surface designs such as central composite or Box-Behnken designs. A comparison of number of runs for mixture design, central composite design and Box-Behnken design for second order model is given at Table 1.

Another advantage of mixture experiments appears when the cost function includes only manufacturing costs. In such cases, the solution of the tolerance allocation problem turns out on the assembly tolerance T. In mixture experiments all of the design points are on the $\sum_{i=1}^{k} x_i = 1$ (i.e., $\sum_{i=1}^{k} t_i = T$), where $x_i = t_i / T$. On the other hand, when response surface designs such as CCD or BBD are used to estimate the cost function, some design points fall outside the plane or prism defined by $\sum_{i=1}^{k} t_i = T$ related to the constraints on the t_is.

BBD and CCD are advantageous designs regarding their orthogonality and rotatability properties, especially when a second order model is used. However, when mixture designs are utilized these advantages diminish because of the component constraints and high linear dependencies can occur. One disadvantage of the linear dependency is the increase in the variance of b_is and $\hat{y}$'s. In order to avoid this undesirable, techniques like best subset selection, stepwise regression, forward elimination, and backward elimination can be employed. By this way model estimates may have better properties. Therefore, predicted cost values may have lower prediction variance when mixture designs are used. An example related to this situation is given in the next section.

When the cost function includes quality loss together with manufacturing cost, the solution of the tolerance allocation problem turns out anywhere on the region defined by $\sum_{i=1}^{k} t_i \leq T$ (i.e., $\sum_{i=1}^{k} x_i \leq 1$). In such cases, if a slack variable is added, the optimum solution turns out on the $\sum_{i=1}^{k+1} x_i = 1$. In this situation, even though the number of components and the number of design points increase, this does not lead to a serious disadvantageous case for k=3 and k=4 shown in Table 1.

Fig. 3 A portion of a steering mechanism

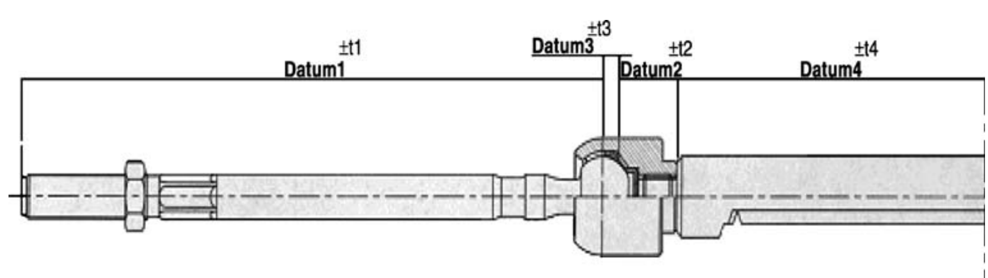

Table 2 The constraints on the component tolerances

Component name	Component code	Minimum tolerance	Maximum tolerance
Datum 1	t_1	0.8 mm	3.2 mm
Datum 1	t_2	0.4 mm	1.2 mm
Datum 1	t_3	0.2 mm	0.2 mm
Datum 1	t_4	0.4 mm	1.2 mm

3.3 An illustrative example

Figure 3 shows an example of a portion of a steering mechanism, which consists of components X_1, X_2, X_3, and X_4. The associated component tolerances are t_1, t_2, t_3, and t_4. The tolerance for assembly is 5.0 mm. The constraints on the component tolerances are given in Table 2. The constrained region, i.e., feasible region, which depends on the constraints on the component tolerances, is drawn in Fig. 4. The objective is to allocate the assembly tolerance optimally between the components X_1, X_2, and X_4 such that the component tolerances give minimum manufacturing cost. In this problem the tolerance for component X_3 is 0.2 mm and fixed. So assembly tolerance can be accepted as 4.8 mm (i.e., $t_1 + t_2 + t_4 \leq 4.8$ mm).

In this example, the extreme vertices design is used to obtain the data. To obtain the design points, approximation function and analysis of variance results, SAS software is used. The associated design points, which are found by using mixture design command in MINITAB and the results of the planned experiments, are given in Table 3. For constructing the mixture design for second order model, "Type of Design" is selected as "Extreme vertices" and "Number of replicates for the whole design" is selected as "2". After the experiments are carried out, resulting cost values are obtained as can be seen in Table 3.

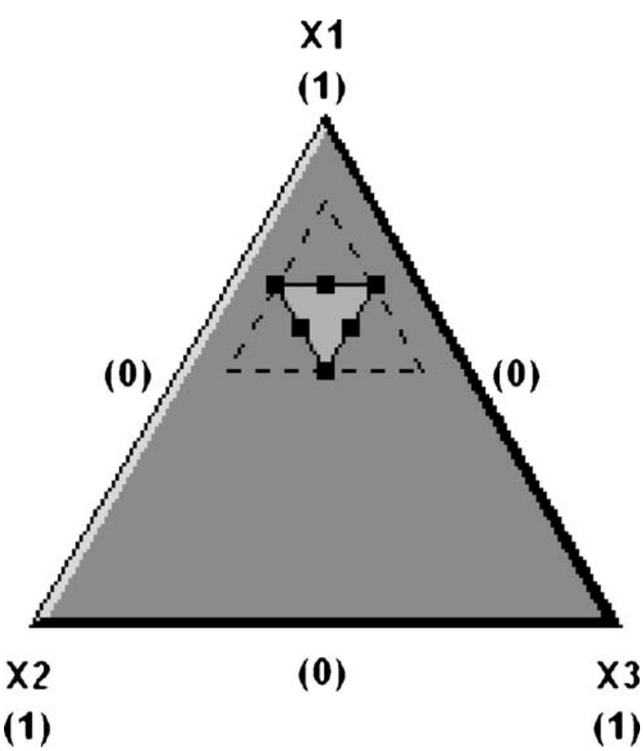

Fig. 4 The constrained experimental region

For full quadratic model in Eq. (8), by using stepwise regression methods, the approximation function is found as

$$\widehat{y} = -51.6x_1 - 82.7x_2 + 90.8x_3 + 445x_1x_2 + 229x_1x_3. \quad (10)$$

The optimum solutions are: x_1=0.6667, x_2=0.2500, x_3=0.0833 (i.e., $t_1^* = 3.2$, $t_2^* = 1.2$, $t_4^* = 0.4$). The predicted manufacturing cost at optimum tolerance solutions is 39.38.

When mixture experiments are used, all of the experimental design points will be on the feasible region. However, when BBD or CCD is used, a number of design points may fall outside of feasible region. When experiments on such points are run, it is also possible to observe some parts that may not be assembled since the total of component tolerances exceeds assembly tolerance.

For the same example, BBD and CCD can also be constructed as it can be seen in Tables 4 and 5. There are some points which exceed the assembly tolerance value for both designs. Feasible region defined by $\sum_{i=1}^{k} t_i = T$ and design points for BBD, CCD and mixture design can be shown in Fig. 5. In addition, it can be seen from Table 5, when CCD and coding formula (4) are used, at axial design points (design points 9–14), individual component tolerance constraints are exceeded. This situation may also lead to functional problems of assemblies. Furthermore, according to design point 9, tolerance of component 1 should have a negative value, which is impossible in practice. When our loss function deals with both manufacturing costs and assembly costs utilization of CCD may not be feasible because assembly tolerances can not be meet for some design points.

A low variance of a predicted value, i.e., Var($\widehat{y}$), is a much desired property of a statistically efficient model. For a tolerance allocation problem, when the cost function includes only manufacturing costs, mixture designs may

Table 3 Experimental design and results of experiments

t_1	t_2	t_4	x_1	x_2	x_3	Y	
						rep1	rep2
3.2	0.4	1.2	0.6667	0.0833	0.2500	45	44
3.2	1.2	0.4	0.6667	0.2500	0.0833	40	39
2.8	1.2	0.8	0.5835	0.2500	0.1665	51	52
3.2	0.8	0.8	0.6667	0.1665	0.1665	42	41
2.4	1.2	1.2	0.5000	0.2500	0.2500	60	61
2.8	0.8	1.2	0.5835	0.1665	0.2500	56	55

Table 4 Box-Behnken design for k = 3

Design point	t_1	t_2	t_4	T	x_1	x_2	x_3
1	2.0	0.8	0.8	3.6	0	0	0
2	2.0	1.2	1.2	4.4	0	1	1
3*	3.2	0.8	1.2	5.2	1	0	1
4	2.0	0.8	0.8	3.6	0	0	0
5	0.8	0.8	0.4	2.0	−1	0	−1
6	3.2	0.4	0.8	4.4	1	−1	0
7	2.0	0.8	0.8	3.6	0	0	0
8*	3.2	1.2	0.8	5.2	1	1	0
9	0.8	0.4	0.8	2.0	−1	−1	0
10	0.8	1.2	0.8	2.8	−1	1	0
11	3.2	0.8	0.4	4.4	1	0	−1
12	0.8	0.8	1.2	2.8	−1	0	1
13	2.0	0.4	1.2	3.6	0	−1	1
14	2.0	0.4	0.4	2.8	0	−1	−1
15	2.0	1.2	0.4	3.6	0	1	−1

*At these points assembly tolerance exceeds 4.8

give a better distribution for prediction variance than CCD and BBD on the assembly tolerance T. In order to explain the case, in our example, some component tolerance values, where the assembly tolerance is always exactly 4.8, are determined and shown in Fig. 6. To explore the prediction variances over the subregion which is illustrated in Fig. 6, the prediction variances on the vertices and edges (i.e., mixture design points), on the centroid of this simplex region, and on the midpoints of the lines between the mixture design points and centroid of the region, are examined. The reason for selecting these points is to investigate their model performances in terms of prediction variances, not just on the border of the feasible region, but also inside and in the center of the area. Prediction variance values ($\mathrm{Var}(\widehat{y})$ / σ^2) and standardized prediction variance values ($N\mathrm{Var}(\widehat{y})$ / σ^2) at these component tolerance values are given in Tables 6 and 7. Here σ^2 is the variance of y's and N is the total number of observations. Models for BBD and CCD are determined as full second order models in order to have best rotatability and orthogonality properties. A second order model with three components is given below:

$$\widehat{y} = b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3 + b_{11}x_1^2 + b_{22}x_2^2 + b_{33}x_3^2. \quad (11)$$

Calculation formulas for prediction variance are given in the Appendix. In this example, for most of the component tolerance values (except design point 3 for both CCD and BBD, and design point 5 for only CCD) mixture design gives lower prediction variance than BBD and CCD. It is a fact that a mixture design augmented with center points gives better results by means of prediction variance, and this fact is obvious regarding the results in the last column of Table 6. In addition, prediction variance values for mixture design are closer to each other. On the other hand, prediction variance values for BBD have a wider spread. For this example, it can be said that, mixture design give a better distribution for prediction variance than BBD and CCD.

4 Further discussion and conclusion

In both Jeang [2] and Kim and Cho [1]'s studies, it is emphasized that, with RSM, optimum component toler-

Table 5 Rotatable central composite design with two center points for k=3

Design Point	t_1	t_2	t_4	T	x_1	x_2	X_3
1	0.8	0.4	0.4	1.6	−1	−1	−1
2	3.2	0.4	0.4	4.0	1	−1	−1
3	0.8	1.2	0.4	2.4	−1	1	−1
4	3.2	1.2	0.4	4.8	1	1	−1
5	0.8	0.4	1.2	2.4	−1	−1	1
6	3.2	0.4	1.2	4.8	1	−1	1
7	0.8	1.2	1.2	3.2	−1	1	1
8*	3.2	1.2	1.2	5.6	1	1	1
9**	−0.01815	0.8	0.8	1.58185	−1.68179	0	0
10*	4.01815	0.8	0.8	5.61815	1.68179	0	0
11***	2.0	0.12728	0.8	2.92728	0	−1.68179	0
12***	2.0	1.47272	0.8	4.27272	0	1.68179	0
13***	2.0	0.8	0.12728	2.92728	0	0	−1.68179
14***	2.0	0.8	1.47272	4.27272	0	0	1.68179
15	2.0	0.8	0.8	3.6	0	0	0
16	2.0	0.8	0.8	3.6	0	0	0

*At these points assembly tolerance exceeds 4.8
**At this point tolerance of component 1 should be a negative number, and practice it's impossible.
***At these points, individual tolerances are either not met or exceed although assembly tolences are met.

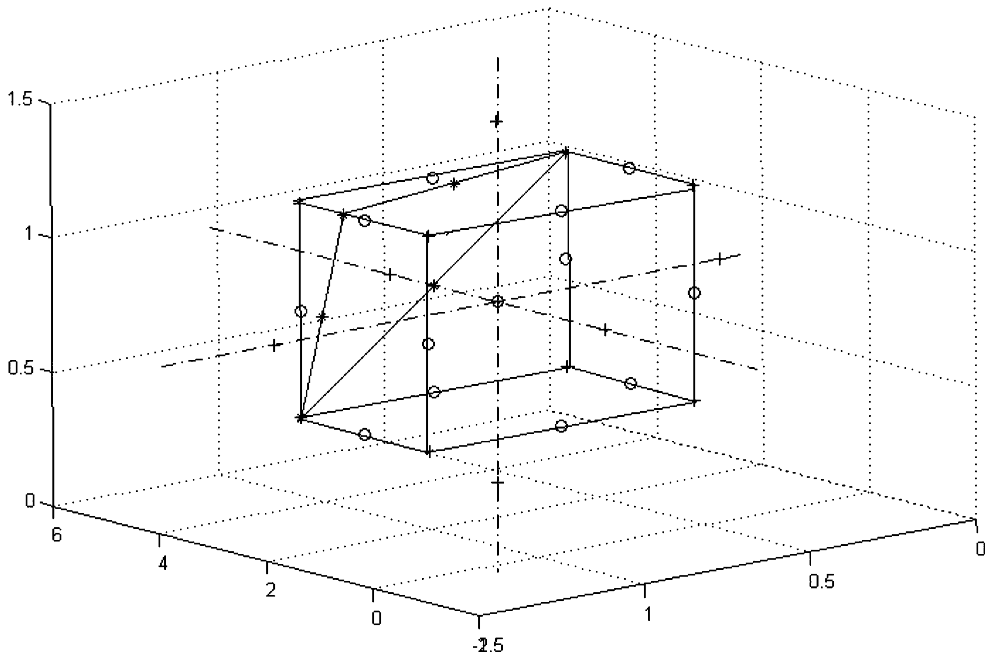

Fig. 5 Experimental design points for BBD,CCD and mixture design and the feasible region defined by $\sum_{i=1}^{k} t_i = T$

ances can be determined, based on the predicted manufacturing cost or total cost values. In their studies, they proposed using the response surface designs such as BBD or CCD to determine predicted cost functions. In this article, the use of mixture designs for tolerance allocation is demonstrated.

There are several advantages of using mixture designs instead of BBD or CCD. First, when mixture designs are preferred, fewer design points are required than are required for BBD or CCD. Second, all design points in the experimental design are on the feasible region. When BBD or CCD is used, some or many of the design points can fall outside of the feasible region. This situation may lead to larger variances of the predicted cost values on a large part of the region defined by assembly tolerance T. Additional constraints at component tolerances can be exceeded which may result in functional problems on assemblies.

Using CCD designs reveals extra disadvantages. When CCD is constructed with the coding formula (4) proposed by Kim and Cho [1], some design points may require negative tolerances as we have seen in illustrative example because of the design parameter constraints on the component tolerances. This problem can be handled in two ways: a coding formula other than proposed by Kim and Cho [1] could be used, or ±α values on axial design points could be chosen as ±1.

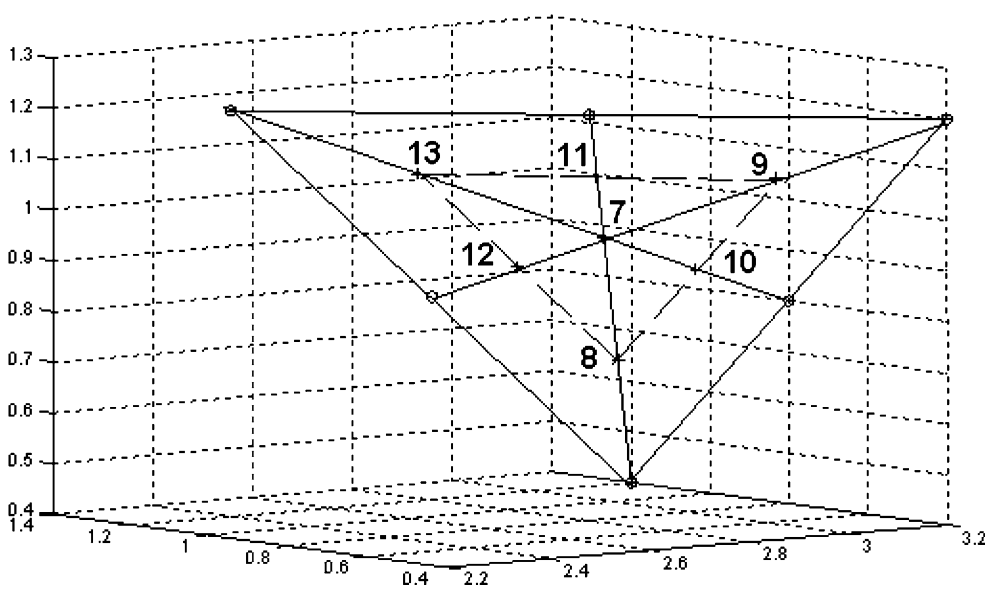

Fig. 6 Some tolerances on the constrained region. °Design points. $^{+}$Some points on feasible region defined by $\sum_{i=1}^{k} t_i = T$

Table 6 Prediction variance values for some component tolerances on the T=4.8 which are presented in Fig. 6

Points	t_1	t_2	t_4	BBD*	ccd*	Mixture design**	Mixture design***
1	3.2	0.4	1.2	1.395833	0.669963	0.415775	0.414732
2	3.2	1.2	0.4	1.395833	0.669963	0.415775	0.414732
3	2.8	1.2	0.8	0.486368	0.337777	0.499983	0.430723
4	3.2	0.8	0.8	0.395833	0.338817	0.168497	0.164732
5	2.4	1.2	1.2	0.572788	0.305065	0.499988	0.49569
6	2.8	0.8	1.2	1.395833	0.669963	0.499983	0.430723
7	2.933	0.933	0.933	0.323123	0.357699	0.208799	0.148669
8	3.0665	0.6665	1.0665	0.496432	0.371957	0.189887	0.15816
9	3.0665	1.0665	0.6665	0.430773	0.339128	0.189887	0.15816
10	3.0665	0.8665	0.8665	0.344872	0.351829	0.134341	0.102569
11	2.8665	1.0665	0.8665	0.329495	0.339445	0.282421	0.212726
12	2.8665	0.8665	1.0665	0.383754	0.366575	0.282421	0.212726
13	2.6665	1.0665	1.0665	0.338936	0.325587	0.222956	0.177377

* For these designs, full second order model, which is defined by Eq. (11) is used
** For this design, model defined by Eq. (10) is used
*** Design which augmented with two center points

Using the mixture designs also reveals some disadvantages. When the linear dependence between the factors is strong, variance inflation factor (VIF) values would be large and predicted cost values would have large variances. To handle this problem, model fitting methods such as stepwise regression, forward elimination or backward elimination can be used.

Appendix

Calculation formulas for prediction variance

In general, predicted tolerance - cost model can be written in matrix notation as,

$$\widehat{y} = Xb \tag{A.1}$$

where $\widehat{y}$ is $N \times 1$ vector of predictor cost values, X is the $N \times p$ matrix representing the design settings used as well as the columns necessary to accommodate the assumed model, and b is a $p \times 1$ vector of estimated coefficients. Let x be an arbitrary point that is located in the design region, and let $f(x)$ the appropriate expansion of x to accommodate the assumed model. The fitted response at the arbitrary point x is given by

$$\widehat{y} = f(x)'b. \tag{A.2}$$

The variance of the predicted response value at the point x is

$$Var(\widehat{y}) = \sigma^2 f(x)'(X'X)^{-1} f(x). \tag{A.3}$$

Table 7 Standardized prediction variance values for some component tolerances on the T=4.8, which are presented in Fig. 6

Points	t_1	t_2	t_4	BBD*	ccd*	Mixture design**	Mixture design***
1	3.2	0.4	1.2	20.9375	10.7194	4.9893	5.806245
2	3.2	1.2	0.4	20.9375	10.7194	4.9893	5.806245
3	2.8	1.2	0.8	7.2955	5.4044	5.9998	6.030119
4	3.2	0.8	0.8	5.9375	5.4211	2.0220	2.306245
5	2.4	1.2	1.2	8.5918	4.8810	5.9999	6.939655
6	2.8	0.8	1.2	20.9375	10.7194	5.9998	6.030119
7	2.933	0.933	0.933	4.8468	5.7232	2.5056	2.081372
8	3.0665	0.6665	1.0665	7.4465	5.9513	2.2786	2.214234
9	3.0665	1.0665	0.6665	6.4616	5.4260	2.2786	2.214234
10	3.0665	0.8665	0.8665	5.1731	5.6293	1.6121	1.43597
11	2.8665	1.0665	0.8665	4.9424	5.4311	3.3891	2.978169
12	2.8665	0.8665	1.0665	5.7563	5.8652	3.3891	2.978169
13	2.6665	1.0665	1.0665	5.0840	5.2094	2.6755	2.483276

* For these designs, full second order model which is defined by Eq. (11) is used
** For this design, model defined by Eq. (10) is used
*** Design which augmented with two center points

Since σ^2 is generally unknown and beyond the control of experimenter, in most study, it is preferred to work with the quantity

$$\frac{Var(\widehat{y})}{\sigma^2} = f(x)'(X'X)^{-1}f(x). \tag{A.4}$$

It is common in RSM to scale criteria such as the prediction variance by the total number of observations, N. Scaled quantity

$$\frac{N \cdot Var(\widehat{y})}{\sigma^2} = N \cdot f(x)'(X'X)^{-1}f(x) \tag{A.5}$$

is also called standardized prediction variance. It is important to note that, the prediction variance depends only on the design points and the form of the assumed model (through $f(x)$) and the specific location of x.

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