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BLOCK DESIGNS FOR MIXTURE EXPERIMENTS

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1. Introduction. Scheffé (1958), (1963) introduced Simplex–Lattice and Simplex–Centroid designs for experiments with mixtures. Recently, Murty (1966) and Murty and Das (1968) have evolved Symmetric-Simplex designs which are the generalized form of Scheffé's designs.

One of the basic requirements for any response surface design according to Box and Hunter (1957) is that it should lend itself to blocking. Mixture designs so far available in literature lack this desirable characteristic. Murty (1966) did make some efforts for blocking the Symmetric–Simplex designs and reached the conclusion which, however, is empirical, saying that the actual blocking is not possible and the only possibility is to replicate the designs. Our investigations into this problem indicate that though the orthogonal blocking ensuring estimation of the regression parameters independent of the block effects is not possible without transforming the mixture variables, yet the parameters can be estimated by adjusting the parameters for the block effects. In the present paper we have derived the conditions required for blocking for estimating the parameters of a quadratic model. We have also constructed designs which satisfy these blocking conditions and hence are amenable to blocking. In the last section we have also constructed orthogonal blocking arrangements through suitable transformations. The case of cubic model will be dealt with in a separate paper.

2. The quadratic model.

2.1. *The blocking conditions.* Let the quadratic model proposed by Scheffé (1958) with block effects be

$$Y_u = \sum_{1 \leqq i \leqq n} \beta_i x_{iu} + \sum_{1 \leqq i < j \leqq n} \beta_{ij} x_{iu} x_{ju} + \sum_{w=1}^{t} \beta_w z_{wu} \tag{2.1}$$

where Y_u represents the response at the uth experimental point; $(u = 1, 2, \cdots, N)$, β_i and β_{ij} are the regression coefficients, x_{iu}'s are the mixture components such that $0 \leqq x_{iu} \leqq 1$ and $\sum_{1 \leqq i \leqq n} x_{iu} = 1$ for each $u = 1, 2, \cdots, N$, β_w is the expected value of the response in the wth block, $w = 1, 2, \cdots, t$ and

$$\begin{aligned} z_{wu} &= 1 \quad \text{for those experimental points which fall in the } w\text{th block} \\ &= 0 \quad \text{for all other points.} \end{aligned}$$

Let the design with t blocks and N experimental points satisfy the following symmetry conditions of Murty and Das (1968):

$$\begin{gathered} \sum x_{iu}^2 = A, \qquad \sum x_{iu} x_{ju} = B, \qquad \sum x_{iu}^2 x_{ju} = C, \\ \sum x_{iu} x_{ju} x_{ku} = D, \qquad \sum x_{iu}^2 x_{ju}^2 = E, \qquad \sum x_{iu}^2 x_{ju} x_{ku} = F, \\ \sum x_{iu} x_{ju} x_{ku} x_{1u} = G \qquad \text{for all} \quad i \neq j \neq k \neq 1. \end{gathered} \tag{2.2}$$

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