

Selection of the Optimal Mathematical Model of Multiple Regression in the Ternary Mixture Experiments

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For a three-component system, regression models can be generally set in the form of polynomials which are usually defined by the following Scheffé canonical forms: a) linear model, b) square model, c) incomplete cube model, d) complete cube model, e) incomplete quartic model, f) complete quartic model. From a lot of models that meet the adequacy requirement it is necessary to choose a model with a rational number of variables for the purpose of easy interpretation and practical application of the model. The paper presents the criteria for evaluation of the model quality and selection of the “optimal” model composition with a “rational” number of variables.

Keywords: Optimal Model, Multiple Regression, Ternary Mixture Experiments

0. INTRODUCTION

Three-component systems can be graphically represented in 2-D space by applying ternary graphs. The main condition for application of ternary graphs is:

$$0 \leq X_i \leq 1; \quad \sum_{i=1}^3 X_i = 1. \quad (1)$$

X_i – the relative proportion of a component in the mixture.

From the previously mentioned conditions, it is noticeable that the proportion of each component in the mixture depends on the proportion of the remaining two components.

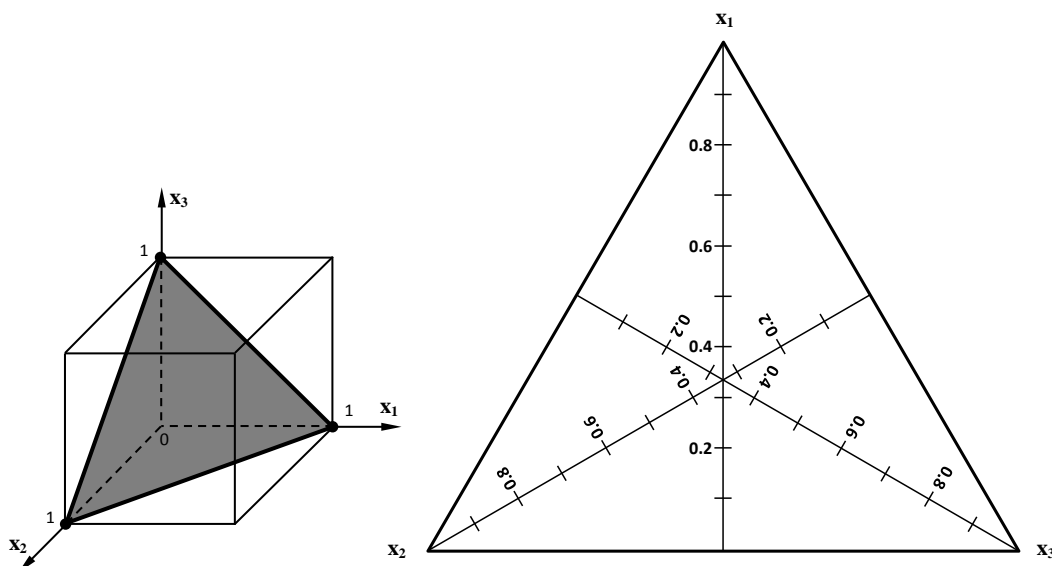


Fig. 1. Triangular (trilinear) coordinate system and representation of vertical sections and the directions of increase in the proportion of individual components

Each point inside the triangle represents a corresponding composition of the three-component system. The vertices of the triangle represent pure substances, while the points on the sides of the triangle represent two-component systems. For a point inside the triangle, the proportion of each component is read by drawing lines through the given point in such a way that they are parallel to the sides of the triangle (Figure 2).

For the three-component system, regression models can be generally set in the form of polynomials which are defined by the following canonical or Scheffé forms [1] [2] [7]:

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