



## APPLICATION OF THE TRIANGULAR COORDINATE SYSTEM FOR CREATION OF PLANE AND SPATIAL TERNARY GRAPHS

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**Abstract:** In the process of investigation of electrical and mechanical properties of alloys, three-component systems play a very important role. Regression analysis provides a possibility to use experimental results in order to obtain the theoretical dependence of these values on the molar ratio of certain components of the mixture. As this refers to multidimensional problems, it is of great importance to present this correlation, in addition to analytical dependencies, by graphical representations. For these needs Draper and Lawrence introduced a new reference system whose base is a concentration triangle ( $X_1$ ,  $X_2$ ,  $X_3$ ) in which the molar ratios of components are drawn on the sides of the equilateral triangle.

The paper shows the process of transformation of values from the triangular system into the Cartesian coordinate system and the executable code for presentation of plane (2D) and spatial (3D) ternary graphs in Matlab.

**Key words:** mixture design, ternary graph, triangular coordinate system

### 1. INTRODUCTION

Three-component systems can be graphically represented in 2-D and 3-D space by applying ternary graphs. The main conditions for application of ternary graphs are:

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

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

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

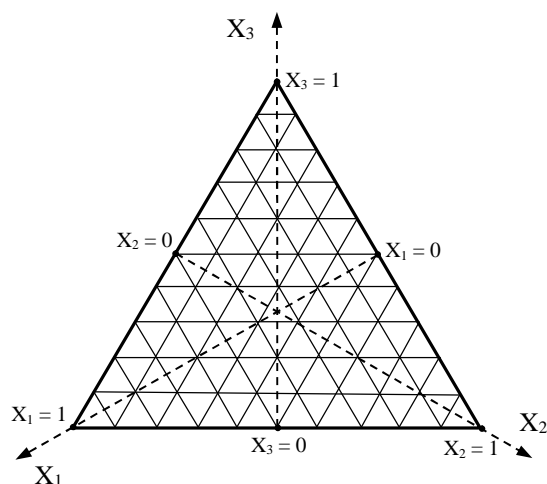


Fig. 1. Vertical sections and directions of increase in the proportion of individual components in the ternary graph

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 up to the remaining two sides of the triangle.

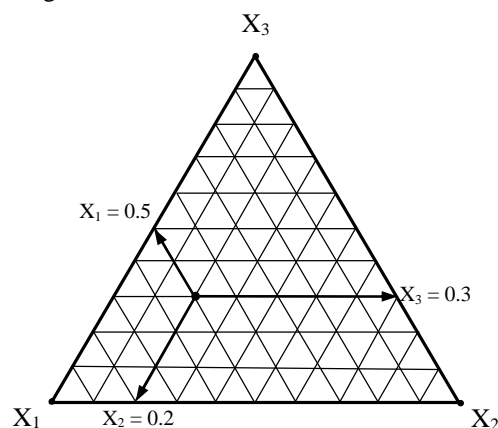


Fig. 2. Determination of the composition of an alloy in the ternary system

### 2. REGRESSION ANALYSIS

In the process of investigation of electrical and mechanical properties of alloys, three-component systems play a very important role. Regression analysis provides a possibility to use experimental results in order to obtain the theoretical dependence of these values on the molar ratio of certain components in the mixture. For the three-component system, in a general case, regression models can be set up in the form of low-degree polynomials

(commonly first, second and third), which are most frequently defined by the following canonical forms [1] [2]:

- Linear regression model

$$y = b_1X_1 + b_2X_2 + b_3X_3 \quad (2)$$

- Quadratic regression model

$$y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 \quad (3)$$

- Special cubic regression model

$$y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{123}X_1X_2X_3 \quad (4)$$

- Full cubic regression model

$$y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{123}X_1X_2X_3 + \delta_{12}X_1X_2(X_1 - X_2) + \delta_{13}X_1X_3(X_1 - X_3) + \delta_{23}X_2X_3(X_2 - X_3) \quad (5)$$

In order to carry out the procedure of regression analysis of the three-component system and make a selection of an adequate regression model, it is necessary to have the following phases [3]:

- Selection of possible forms of regression models
- Calculation of regression coefficients
- Checking the adequacy of mathematical models
- Selection of the regression model
- Evaluation of the significance of regression coefficients of the selected model
- Calculation of confidence limits of regression coefficients of the selected model
- Graphical interpretation of the mathematical model

### 3. CREATION OF A TERNARY GRAPH

As these problems are multidimensional, it is of great importance to present this correlation, in addition to analytical dependencies, by graphical representations. For these needs, Draper and Lawrence[2] introduced a new reference system whose base is a concentration triangle ( $X_1, X_2, X_3$ ) in which the molar ratios of components are drawn on the sides of the equilateral triangle.

There is a multitude of software for drawing graphs in the triangular system. However, for the needs of its own research, the Faculty of Mechanical and Civil Engineering in Kraljevo has developed software for regression analysis of three-component systems RA-TeS v1.1 (Regression Analysis in Ternary System). Besides, the program package Matlab has been used to develop the procedure of obtaining a 3D surface graph and a 2D contour graph in the triangular coordinate system. The possibility of obtaining such a graphical representation gives a clear picture and enables easy interpretation of dependence of the observed characteristic on dependent variables in the ternary system.

The continuation of the paper presents the procedure of conversion of values from the triangular into the Cartesian

coordinate system and the executable code for presenting planar (2D) and spatial (3D) ternary graphs in Matlab.

The function  $Z$  depends on the variables  $X_1, X_2, X_3$ . In order to draw its values into the ternary graph, the program should convert the values  $X_1, X_2, X_3$  from the triangular system into the Cartesian coordinates  $X$  and  $Y$ . Draper and Lawrence[2] placed the Cartesian coordinate XYZ system into the centre of the equilateral triangle ( $X_1, X_2, X_3$ ), which is in the plane  $XY$ . The relation between the coordinates is expressed by the following dependencies:

$$\left. \begin{aligned} X &= \frac{1}{2}(-X_1 + X_2) \\ Y &= \frac{\sqrt{3}}{6}(-X_1 - X_2 + X_3) \end{aligned} \right\} \quad (6)$$

$$\left. \begin{aligned} X_1 &= \frac{1}{3}(-3X - Y\sqrt{3}) \\ X_2 &= \frac{1}{3}(3X - Y\sqrt{3}) \\ X_3 &= \frac{1}{3}(2Y\sqrt{3}) \end{aligned} \right\} \quad (7)$$

For the needs of this paper, the X-axis of the Cartesian coordinate system is perpendicular to the axis  $X_1$  and coincides with the base of the triangle which passes through the vertices  $X_2$  and  $X_3$ . The coordinate beginning is placed at the vertex of the triangle  $X_2$  (Figure 3).

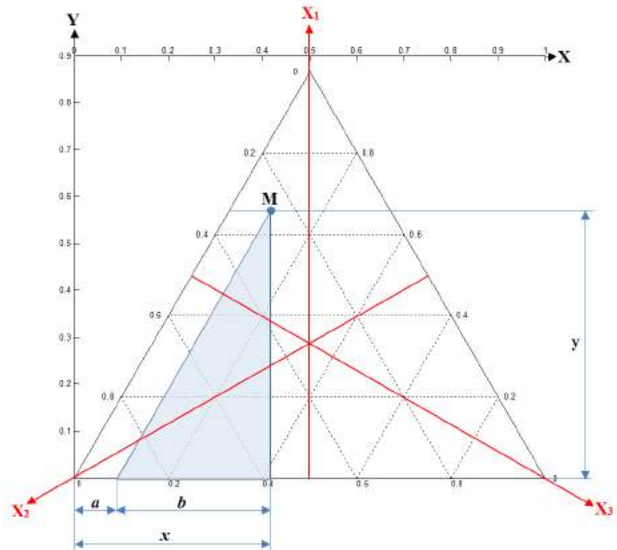


Fig. 3. Correlation between Cartesian coordinates and coordinates in the concentration triangle

The relation between the Cartesian coordinates  $XY$  and the coordinates  $X_1, X_2, X_3$  is expressed by the dependencies:

$$\left. \begin{aligned} Y &= \frac{\sqrt{3}}{2} X_1 \\ X &= X_3 + \frac{1}{2} X_1 \end{aligned} \right\} \quad (8)$$

Although the axes  $X_1$  and  $Y$  are parallel, for correct conversion it is necessary to multiply the values  $X_1$  by  $\frac{\sqrt{3}}{2}$ . The relation between the  $X$  coordinate and the coordinates of the triangle  $X_1, X_2, X_3$  can be found from Figure 3, i.e.

$$\begin{aligned} a &= X_3 \\ b &= \frac{y}{\sqrt{3}} \\ X &= a + b = X_3 + \frac{1}{2} X_1 \end{aligned} \quad (9)$$

Based on the dependency (8), it is possible to write a code in Matlab for drawing a ternary contour graph in the plane or a ternary surface graph in space. The input data for the values  $X_1, X_2, X_3$  and the values of the function  $Z$  are entered in the form of row matrix, and the executable code of the program for drawing graphs reads:

```
%input data
L=[0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]
x1=[0.00 0.10 0.20 0.30 0.40 0.50 0.60
0.70 0.80 0.90 1.00 0.50 0.45 0.40
0.35 0.30 0.25 0.20 0.15 0.10 0.05
0.00 0.50 0.45 0.40 0.35 0.30 0.25
0.20 0.15 0.10 0.05 0.00]
x2=[0.50 0.45 0.40 0.35 0.30 0.25 0.20
0.15 0.10 0.05 0.00 0.00 0.10 0.20
0.30 0.40 0.50 0.60 0.70 0.80 0.90
1.00 0.50 0.45 0.40 0.35 0.30 0.25
0.20 0.15 0.10 0.05 0.00]
x3=[0.50 0.45 0.40 0.35 0.30 0.25 0.20
0.15 0.10 0.05 0.00 0.50 0.45 0.40
0.35 0.30 0.25 0.20 0.15 0.10 0.05
0.00 0.00 0.10 0.20 0.30 0.40 0.50
0.60 0.70 0.80 0.90 1.00]
Z=[132 46 52 87 45.9 45 51.5 56.1 49.7
52 412 32 25.3 42 46 79.6 83 77.3 87
85.7 48.6 294 82 56.4 32.1 30.6 49.7
53.2 67.2 74.8 89.7 88.2 94.2 ]
Z=Z./100
```

```
%vertices of triangle in Cartesian
system
xb=[0 0.5 1 0]
yb=[0 sqrt(3)/2 0 0]
zb=[0 0 0 0]
```

```
%conversion of values from triangular
into Cartesian coordinate system
X=x3+1/2*x1
Y=x1*sqrt(3)/2
```

```
%drawing points in the plane
figure
ternplot(x1, x2, x3, 'k. ');
ternlabel('X1', 'X2', 'X3');

%drawing contour graph
figure
terncontour(x1, x2, Z1);
ternlabel('X1', 'X2', 'X3');
h_ob=findobj(gcf, 'Type', 'hggroup');
set(h_ob, 'LevelStep', 0.2);
set(h_ob, 'ShowText', 'On');
set(h_ob, 'LineWidth', 2)
set(h_ob, 'LevelList', [0.2 0.4 0.6 0.8
1 1.2 1.4 1.6 1.8 2 2.2 2.4 2.6]);

%drawing spatial graph
figure
hold on
plot3(xb,yb,zb, 'k-')
plot3(X,Y,L, 'k. ')
plot3(X,Y,Z, 'k. ')
ternsurf(x1, x2, Z1); ternlabel('X1',
'X2', 'X3');
terncontour(x1, x2, Z1)
h_ob=findobj(gcf, 'Type', 'hggroup');
set(h_ob, 'LevelStep', 0.2);
set(h_ob, 'ShowText', 'On');
set(h_ob, 'LineWidth', 2)
set(h_ob, 'LevelList', [0.2 0.4 0.6 0.8
1 1.2 1.4 1.6 1.8 2 2.2 2.4 2.6]);
hold off
colormap gray
```

The contour and spatial ternary graphs obtained by the above described procedure are shown in Figures 4 and 5.

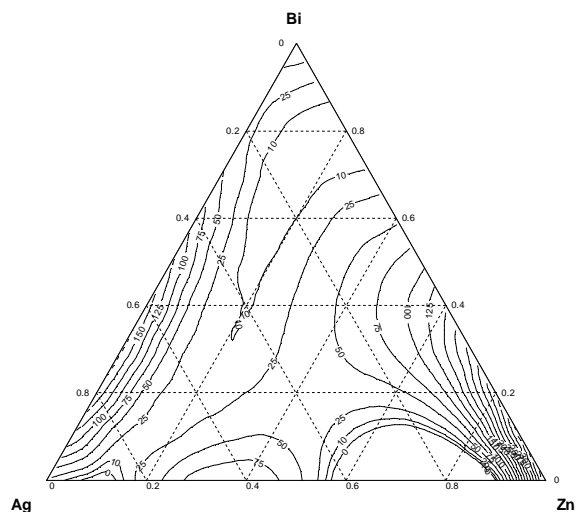


Fig. 4. Ternary contour graph

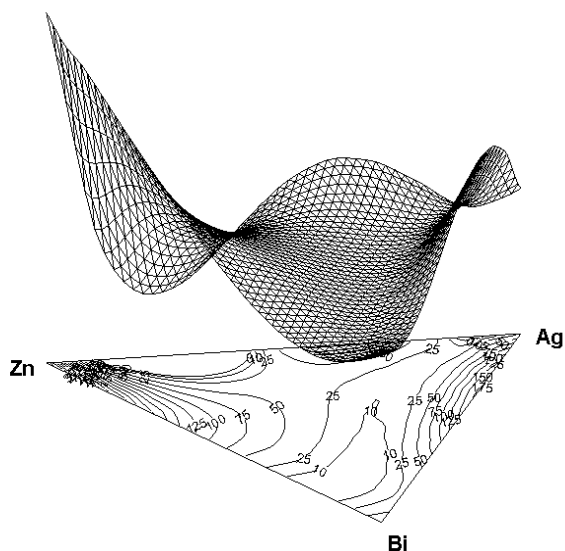


Fig. 5. Ternary spatial graph

The relation and position of the triangular coordinate system in the Cartesian coordinate system can be seen in Figures 6 and 7.

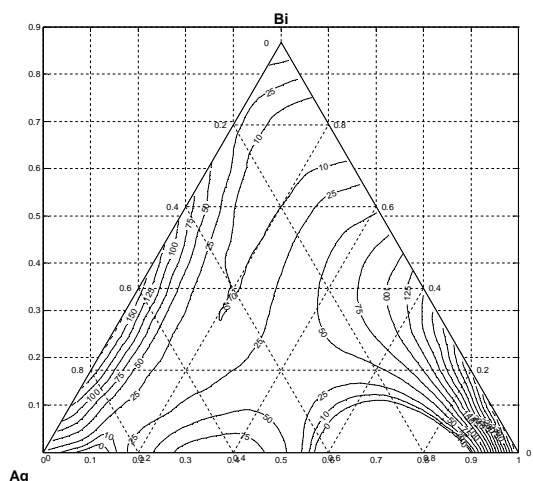


Fig. 6. Position of the contour graph in the Cartesian system

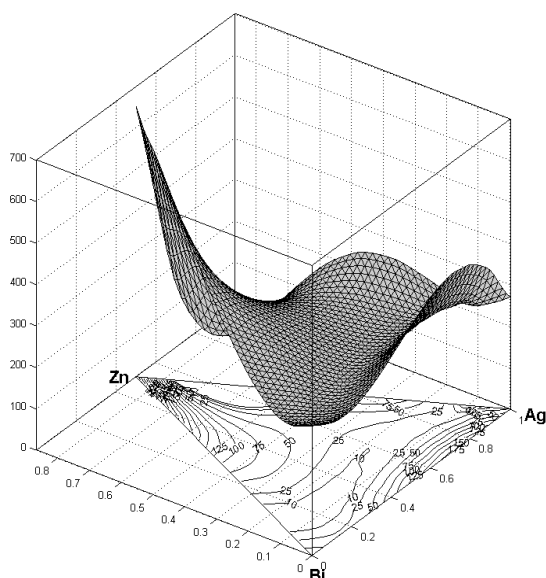


Fig. 7. Position of the spatial ternary graph in relation to the Cartesian system

## 4. CONCLUSION

The theoretical dependence of the observed characteristic of the three-component alloy on the molar ratio of individual components in the mixture, which is obtained by regression analysis after experimental investigation, is more complete when it is possible to have graphical representation of this dependence. These graphs give a clear visual representation and provide easy interpretation of dependencies of the observed characteristic on dependent variables in the three-component system. Ternary graphs are more convenient than contour and spatial graphs because contour and spatial graphs can be used for presentation and analysis of four-dimensional problems, and categorized ternary graphs can be used even for five-dimensional problems.

There is a multitude of software for drawing graphs in the triangular system. However, most of them have limited capabilities for presentation of the obtained graphs. The advantages of developing ternary graphs in Matlab are: it is possible to adjust the look of the graph, the thickness and shape of the lines, select the combination of colours for presentation of lines and surfaces, the manner of writing data on the graph as well as the type and position of the legend, rotate the graph in space for the purpose of selecting the best view, change the mesh density for presentation of isolines or isosurfaces, etc.

These possibilities offered by Matlab are of great importance because, in addition to the obtained mathematical dependencies of the observed characteristics of three-component alloys, they provide such a method of presentation that can be used by scientific institutions for the purpose of easier interpretation of certain phenomena.

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