# MODEL ANALYSIS BY WOLFRAM *MATHEMATICA* FOR COMPOSITION-PROPERTY STUDIES IN MULTICOMPONENT SYSTEMS

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It is known that the state diagrams studies in multicomponent systems are the complicated and labour consuming task. Usually, in the course of the composition-property investigation, experimental data are known only for some local areas and not for the whole composition field. In this connection, for studies of regularities in homogenous systems, design of experiments is often used, which enables one to simplify significantly the investigation process and to represent, at the same time, an adequate mathematical description of the response surface, provided the property under investigation is a continuous function of arguments and it may be represented with necessary precision as the reduced *n*-order polynom [1].

The aim of the current work is in application of the **Wolfram *Mathematica*** [2] package for the solubility experimental data processing using the Scheffe simplex lattice design [3].

The homogeneous areas in the **$LnI_3$ – L – $H_2O$** (Ln = La-Lu; L – organic ligand) ternary systems have been considered as an example, planning matrices and polynomial equations of different orders being constructed for the solubility description of complex compounds, which are formed in these systems, as a function of composition. The adequacy of the equations obtained has been checked with control points. The universal program which allows applying the simplex lattice design to a great number of multicomponent systems, representing polynoms in analytical form, and visualizing the respective response surfaces has been developed. The regularities in the solubility change along the lanthanides row and its decrease with the ligand concentration growth has been clearly demonstrated.

## References

*1. Scheffe H.* Simplex – centroid design for experiments with mixtures // *J. Roy. Statist. Soc. B* **25,** 1963. P. 235-263.
2. http://www.wolfram.com/mathematica
3. *Akhnazarova S.L., Kafarov V.V.* Optimization of experiments in chemistry and chemical technology. Moscow, Vysshaya shkola, 1978. 319 pp. (Russian.).