CONSTRUCTION OF EXCESS GIBBS ENERGY DIAGRAMS FOR FOUR-COMPONENT SYSTEMS USING THE MARCHING CUBES ALGORITHM

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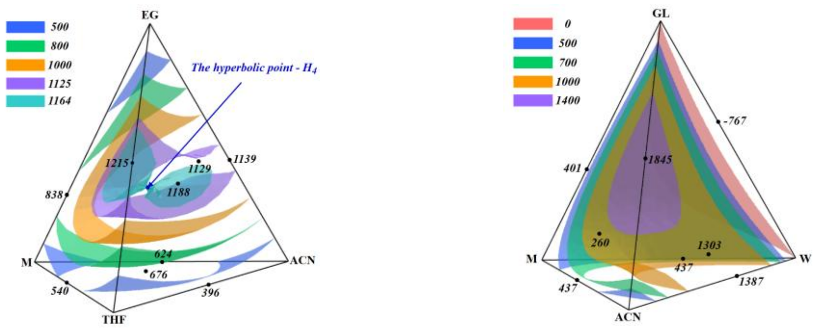
Using the «marching cubes» algorithm, the visualization of datasets representing composition – excess Gibbs energy for four-component systems methanol (M) – tetrahydrofuran (THF) – acetonitrile (ACN) – ethylene glycol (EG) and methanol (M) – acetonitrile (ACN) – water (W) – glycerol (GL) was performed at a pressure of 101.32 kPa. Calculations were carry out using the Non Random Two Liquid (NRTL) model, which allows describing the concentration dependencies of G^E in binary systems with different deviations from ideal behavior, as well as structures of G^E diagrams with several inner singular points [1].

In figure, the arrangement of iso-manifolds of excess Gibbs energy (G^E) is shown in concentration tetrahedrons of four-component systems. For the G^E structures of the ternary diagrams, the conditions of topological verification are satisfied for the complete systems: $2E_3 + E_2 + E_1 = 2H_3 + H_2 + 2$, where E – elliptic point; H – hyperbolic point; 1, 2, 3 – the number of components in singular point. Furthermore, the condition holds for the boundary contour: $E_2^{max} + H_2^{max} + E_1^{max} = E_2^{min} + H_2^{min} + E_1^{min}$, where the numbers of binary singular points with maximum (max) and minimum (min) values of G^E on the binary systems are equal [1,2].

The application of the marching cubes algorithm allows determining the compositions of G^E for four-component singular points, which significantly simplifies the analysis of G^E diagrams when studying solution structure and extractive agents selectivity for separating ternary mixtures with multiple azeotropes.



The iso-manifolds of the excess Gibbs energy (J/mol) of M-THF-ACN-EG and M-ACN-W-GL mixtures at a pressure of 101,32 kPa

1. Raeva V. M. Russ. J. Phys. Chem. A. 2015. 89 (8). Pp. 1316-1324.
2. Serafimov L.A., Raeva V.M., Stepanov V.N. Theor.Found. Chem. Eng. 2012. 46 (3). P. 221-232.