SIMPLIFIED PROCEDURE FOR ANALYZING VAPOR-LIQUID EQUILIBRIUM DIAGRAMS OF MULTICOMPONENT SYSTEMS

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The study of VLE diagrams of multicomponent systems is a rather difficult task. Well-known methods involve the graphical construction of a boundary or complete phase space, the construction and analysis of adjacency and reachability matrices. In some cases, this procedure can be simplified; in particular, when azeotropes relative to the constituents of the same component number are nodal points [1-2].

The initial information is data on the boiling points (BP) of all singular points. Let's illustrate specifics mentioned and stages of VLE diagram analysis using the example of a methanol (M) + ethanol (E) + ethyl acetate (EA) + toluene (T) + hexane (N) system. BP, type and Poincare index (PI) are given in the tables.

Boiling points and types of singular points ($N^{(un)st}$ – (un)stable node, S – saddle)

Sing. point	**M**	**E**	**EA**	**T**	**H**	**M+H**
BP, °C	64.53	78.31	77.20	110.68	68.73	50.98
Type (PI)	S (0)	N^{st} (+1)	S (0)	N^{st} (+1)	S (0)	N^{un} (+1)
Sing. point	**M+T**	**E+H**	**EA+H**	**E+EA**	**M+EA**	**E+T**
BP, °C	63.60	58.37	65.37	72.02	62.52	76.96
Type (PI)	S (0)	S (0)	S (0)	S (0)	S (0)	S (-1)

There are 4 edges adjacent to the vertex of each singular point, comparing the boiling points, it is possible to determine the type of points at the vertex (table). There will always be one unstable node in systems of type considered; it is azeotrope M+H. By solving the following equation [2], the number of binary saddles with a nonzero Poincare index can be determined:

$$2N_5^+ + N_4^+ - C_4^- + N_3^+ + C_3^+ + N_2^+ - C_2^- + N_1^+ = 2$$

The terms $N_5^+, N_4^+, C_4^-, N_3^+, C_3^+$ are equal to zero due to the absence of such points, $N_2^+ = 1$, $N_1^+ = 2$, so $C_2^- = 1$. The system contains one binary azeotrope of the saddle type with index -1 that can be formed only by points of pure components of the stable node type, i.e. azeotrope E+T. The latter will generate an internal separatric hypersurface of the third dimension (SH_3). The remaining singular points are saddles with zero index. Such binary azeotropes will generate separatric manifolds, but of a smaller dimension, which will form a boundary surface of SH_3. SH_3 separates diagram into two distillation regions. Thus, the complete structure of the composition pentatope is determined only based on qualitative analysis.

1. A.V. Frolkova. *Theor. Found. Chem. Eng*. 2024, 4, 1017.
2. A.V. Frolkova, etc. *Theor. Found. Chem. Eng*. 2025, 3, 23.