

**MULTICOMPONENT SYSTEMS SIMULATION
BY THE SOFTWARE OF "DIAGRAMS DESIGNER"**

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Abstract

Method to model the T-x-y and T-x-y-z diagrams by means of kinematically produced surfaces and hypersurfaces has been considered. The models of T-x-y diagram with an eutectical solubility gap, its topological modifications, horizontal and vertical sections are considered. The principles of T-x-y-z diagrams simulation are presented using T-x-y-z diagram with the two eutectical solubility gaps.

The elaboration of phase diagrams computer simulation methods and the attendant software makes it possible to obtain the visual models of different topology T-x-y and T-x-y-z diagrams and to carry out their thorough investigation by the horizontal and vertical sections building, the conjugate compositions and the crystallization paths calculations, the analysis of three-phase transformation type changing, etc. In parallel with the thermodynamic simulation methods development [1-3] the problem of spatial diagrams computer work models elaboration is actual also. Work models of phase diagrams give the possibility to work with physics-chemical systems on all stages of their studies. In the case of deficiency in necessary experimental or calculation information the different mathematical models can be used.

At the choice of mathematical method to describe the phase regions boundaries in diagrams of any complexity and topological types, the models using minimum of initial experimental data are preferred. A kinematical method of phase diagrams surfaces and hypersurfaces description is the most potential [4-5]. In the case of T-x-y diagram, any surface is presented as the pseudo-ruled one, that is, a space curve, given by the interpolation polynomial, moves along the analogously given directing curves. For T-x-y-z diagrams, the hyper-surfaces are formed by the originating curves moving along the directing surfaces. Such method permits to simulate the phase regions boundaries of any complexity, including the surfaces and hyper-surfaces with extreme points, solubility gaps, folds and closed surfaces using the minimum of initial experimental information. The surfaces and hyper-surfaces having large quantity of points on the contour are formed from the separate fragments or using the additional directing curves building.

1. VARIANTS OF T-X-Y DIAGRAMS RULED AND UNRULED SURFACES DESCRIPTIONS

The ruled surfaces with rectilinear directing lines including four points on contour (fig. 1a) are formed by the originating line moving between the position ac and bd along the two rectilinear directing lines ab and cd. In the general case it is the hyperbolical paraboloid (skew plane), in the particular case it is the plane. The assignment of the additional points on the directing lines permits to obtain the ruled surfaces with curvilinear directing lines (fig. 1b). The quantity and arraignment of additional points define the view and curvature of directing lines. It is suggested that originating segment is degenerated in a points at the construction of surfaces with three points on contour.

In a general way at the surfaces simulation the originating curve is given by the interpolation polynomial of second or higher power and one or several additional directing lines are given within surfaces. For example at smooth surface simulation (fig. 1c) the originating line is moving from position ac to bd along the three directing curves $a(a,b)b$, $e(e,f)f$ и $c(c,d)d$, each of them passes through three points.

A saddle surface of the form as fig. 1d is obtained by the originating line shifting from positions a_1c_1 to point a_6 along the three directing curves given by five points. In a similar way the cupola-shaped surfaces can be formed by the originating line of second degree gliding along the three directing lines. In this case the limited directing lines a_1a_3 and c_1c_3 pass through three points and the intermediate directing curve is formed by five points (fig. 1e). The complexity surfaces including solubility gaps and large quantity of points on the contour are constructed from separate fragments. So the surface with smoothness gap ee_1 (fig. 1f) have five singular points on contour and so it is formed by three fragments.

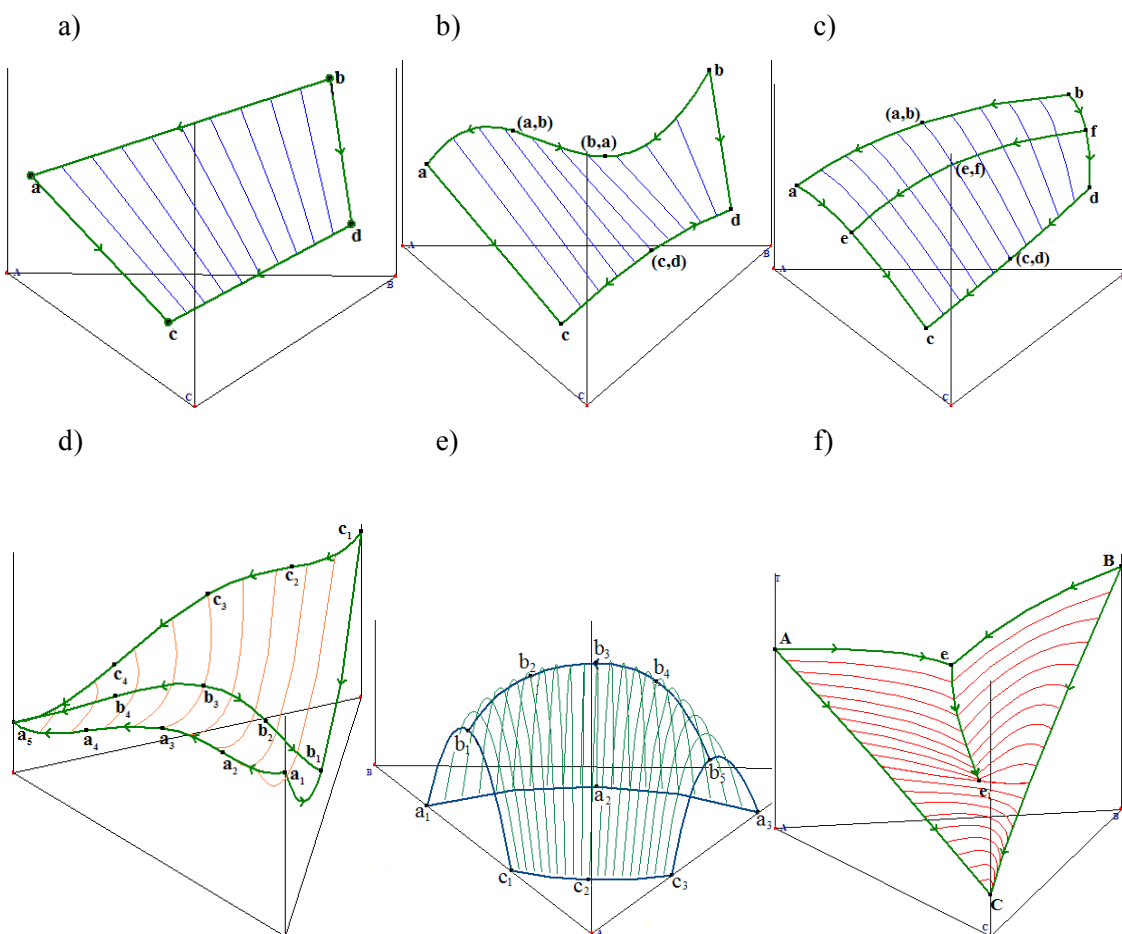


Fig. 1. Kinematical models of ruled surfaces with rectilinear (a) and curvilinear (b) directing lines, surfaces with curvilinear perimeter (c), saddle (d), cupola-shaped (e) and fragmented (f) surfaces

Let's consider suggested method using T-x-y and T-x-y-z diagrams as examples.

2. T-X-Y DIAGRAM WITH ONE EUTECTIC SOLUBILITY GAP MODEL

Given T-x-y diagram include three unruled surfaces (liquid with fold (Q), solidus (S) and solvus (V)) and three ruled surfaces (Q_A^r , Q_B^r and S^r). At that the point on eutectic line end conforms to both maximum and minimum on the monovariant lines. We consider in some detail the first case (fig. 2a) [6 (P. 82), 7 (P. 165), 8 (P. 239)]. The unruled surfaces are formed by the moving of originating curves of second power along the three directing lines passing through three points. The exception is the solvus cupola-shaped surface, its directing lines pass through three, four and five points.

The points corresponding the melt temperature of initial components A, B and C on the prism edges, the end points of eutectic curve e and e_1 , the solvus points on the prism side a, b, a_1 , b_1 and within prism c, c_1 are given as an initial data. The additional points are used for the surface curvature determination (on the contour of surfaces and within the one) and the provision of smoothness on one surface fragments boundaries (table 1).

Table 1

a) Compositions and temperatures of initial points on surfaces contour

Symbol	z_1	z_2	z_3	T	Symbol	z_1	z_2	z_3	T
A	1	0	0	720	a_1	0.84	0.16	0	0
B	0	1	0	550	b	0.18	0.82	0	420
C	0	0	1	1000	b_1	0.12	0.88	0	0
e	0.49	0.51	0	420	c	0.5 originating parameter			
e_1	0,5 originating parameter				c_1	0.26	0.17	0.59	0
a	0.78	0.22	0	420					

b) Coordinates of additional points determining the surfaces curvature

Symbol	z_1	z_2	z_3	T	Symbol	z_1	z_2	z_3	T
(1)	0.8	0	0.2	780	(8)	0	0.48	0.52	780
(2)	0.9	0.31	0	580	C-c	0,18	0,14	0.68	870
(3)	0.27	0.73	0	510	(5)-c	0,75 originating parameter			
(4)	0	0.58	0.42	780	(8)-c	0,25 originating parameter			
e- e_1	0.44	0.43	0.13	620	(6)-[(5)-c]	0,72	0,1	0.18	670
C- e_1	0.19	0.18	0.63	890	(7)-[(8)-c]	0,12	0,63	0.25	640
(1)- e_1	0,75 originating parameter				(9)	0.82	0.18	0	230
(4)- e_1	0,25 originating parameter				(10)	0.15	0.85	0	230
(2)-[(1)- e_1]	0,65	0,27	0.08	690	(11)	0.44	0.11	0.45	280
(3)-[(4)- e_1]	0,23	0,63	0.14	650	(12)	0.18	0.37	0.45	280
(5)	0,71	0	0.29	780	a-c	0,56	0,19	0.25	640
(6)	0.71	0	0.29	780	b-c	0,21	0,53	0.26	630
(7)	0,1	0,9	0	470					

The liquids surface has smoothness gap and therefore it is constructed from three parts (fig. 2b). The moving of originating line from Ae to (1) e_1 along the directing curves ee_1 , (2)(1)- e_1 and the part A(1) of directing curve A(1)C forms the fragment A ee_1 (1). In fragment B ee_1 (4) the directing lines arranges

the limited positions Be and $(4)e_1$ and moves along the directresses ee_1 , $(3)(4)-e_1$ and the part $B(4)$ of directing curve $B(4)C$. The generating fragment $C(1)(4)$ is shifted from $(1)e_1(4)$ to C along the directing lines $(1)C$, $(4)C$ and $e_1(C,e_1)C$. As the directing lines of these liquids fragments are the parts of common lines for all surfaces then the surface smoothness is assured besides the fold ee_1 .

The solidus surface has six singular points on contour and consists of three parts (fig. 2c). The fragment $C(5)(8)$ is formed by the directing lines moving from the position $(5)(8)$ to points C along the lines $(5)C$ and $(8)C$ of directing lines $A(5)C$ and $B(8)C$, and the directing line cC . The originating line of $Aac(5)$ surface fragment arranges the limited positions Aa and $(5)c$ and shifts along the part ac and $A(5)$ of directing lines AC and acb , and the directing curve $(6)(5)-c$. The fragment $Bbc(8)$ is constructed by the gliding of originating line from Bb to $(8)c$ along the line bc and $B(8)$ of directing lines abc and $B(8)C$, and the directing line $(7)(8)-c$. The solvus surface (fig. 1d) is formed by the moving of originating line from aa_1 to bb_1 along the directing lines acb , $(9)(11)(12)(10)$ and $a_1c_1b_1$ given from five, four and three points correspondingly.

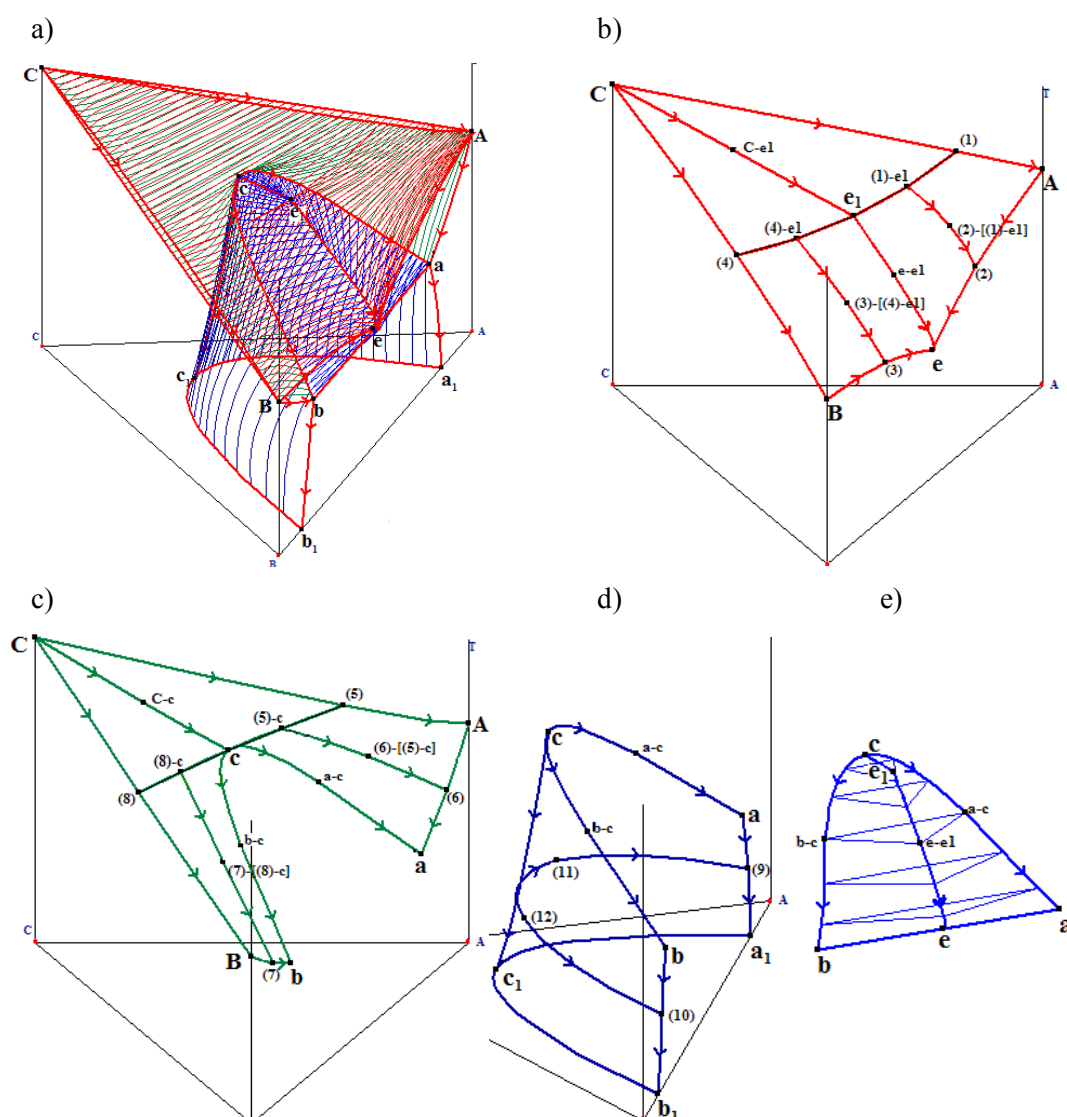


Fig. 2. T-x-y diagram with one eutectic solubility gap (a), the surfaces models of liquids (b), solidus (c), solvus (d) and ruled surfaces (e)

At the ruled surfaces simulation Q_A^r , Q_B^r and S^r the originating segment shifts along the two directing lines. The ruled surface Q_A^r is simulated by the segment ae moving along the line ac and ec , the ruled surface Q_B^r is formed by the gliding of segment eb along the directing curves ec and bc , the moving the segment ab along the curves ac and bc gives the ruled surface S^r .

As a result the model of T-x-y diagram with one eutectic solubility gap is produced. For given model the different horizontal (fig. 3a-c) and vertical (fig. 3d-f) sections can be obtained.

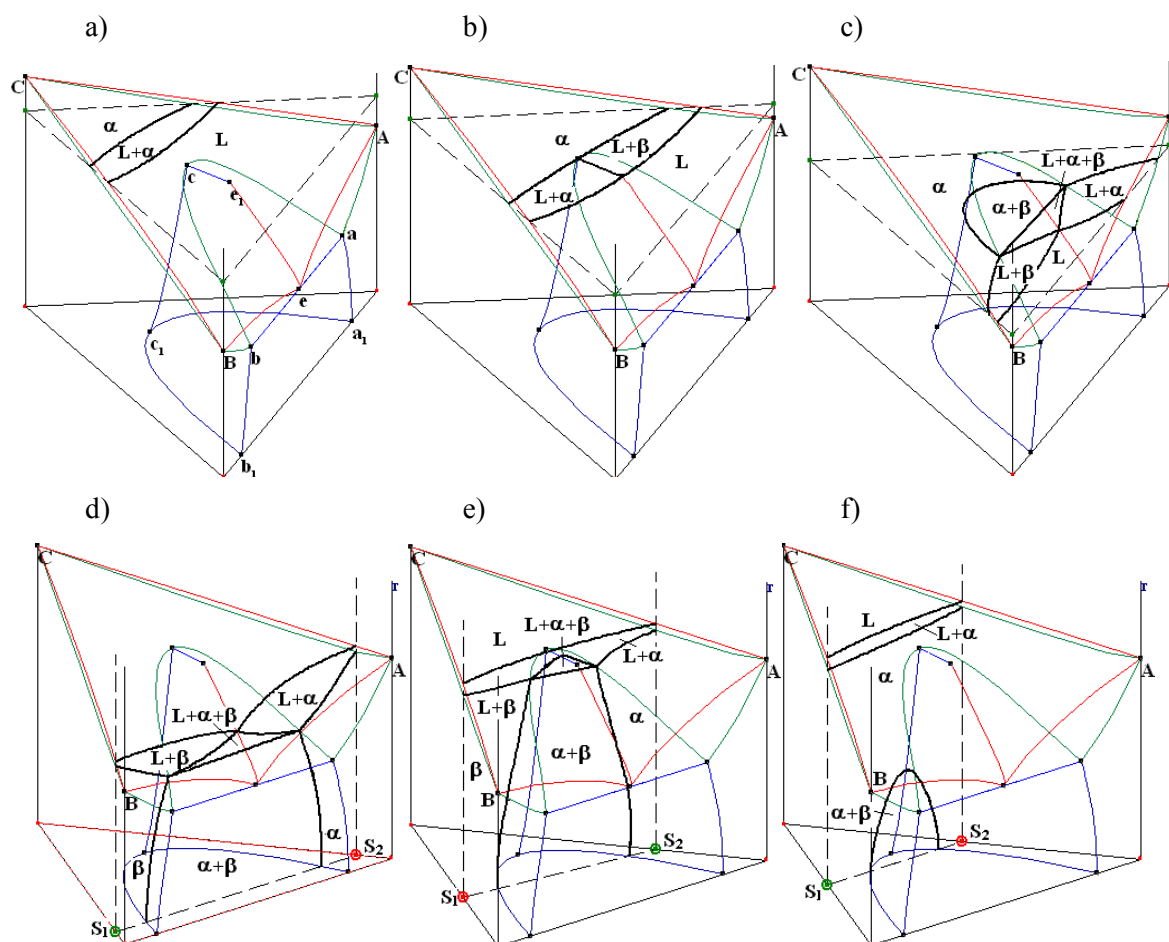


Fig. 3. Horizontal sections at $T_{sech} > T_{e1}$ (a), $T_{sech} = T_{e1}$ (b), $T_{sech} < T_{e1}$ (c); vertical sections $S_1(0; 0.9; 0.1)$ $S_2(0.9; 0; 0.1)$ (d), $S_1(0; 0.6; 0.4)$ $S_2(0.7; 0; 0.3)$ (e), $S_1(0; 0.5; 0.5)$ $S_2(0.5; 0; 0.5)$ (f),

The different modification of given topological type can be obtained on the basis of formed phase diagram model. For example, the variant of T-x-y diagram model with minimum on the monovariant lines at that the eutectic curve intersects the intersection line of solidus and solvus acb in projection was simulated (fig. 4a) [6 (P. 132), 7 (P. 149), 9 (P. 107)]. For given case the problem of changing of three-phase transformation type is fully considered [10], and the surfaces corresponding the changing of three-phase transformation type is constructed (fig. 4b) and the mass balance diagrams are calculated (fig. 4c).

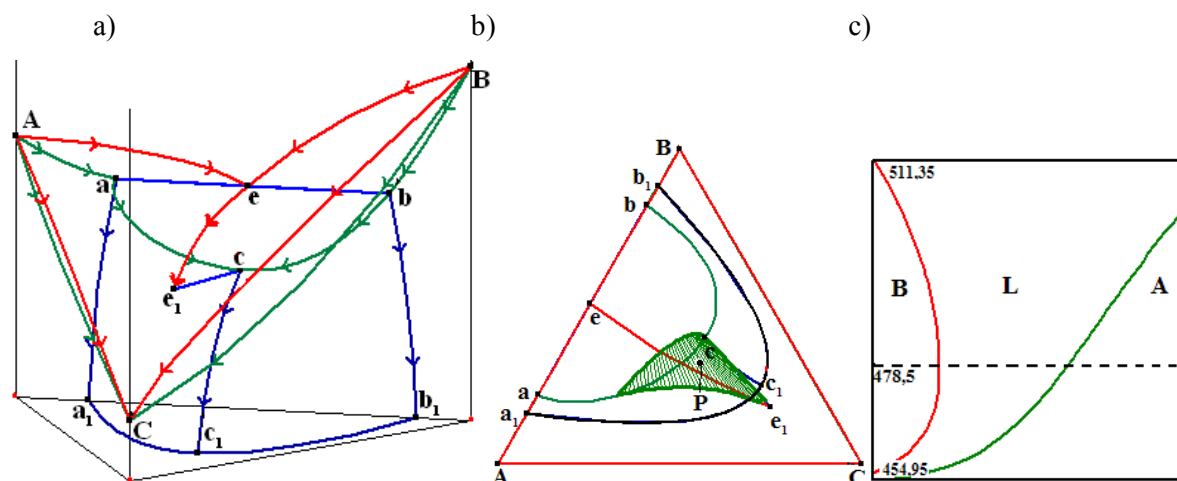


Fig. 4. T-x-y diagram model with the minimum points on monovariant lines (a), the surface of sign mass increasing changing (b) and mass balance for point P (0.28; 0.31; 0.41) (c)

In a similar way the T-x-y diagrams models with one peritectic solubility gap and the points of minimum or maximum on the monovariant line can be simulated and studied [6 (P. 105), 7 (P. 168), 10 (P. 266)].

3. T-X-Y-Z DIAGRAMS MODELS WITH EUTECTIC SOLUBILITY GAPS

T-x-y-z diagram with one eutectic solubility gap has two T-x-y diagrams of similar topological types and two T-x-y diagrams with the continuous range of solid solution on their boundaries. This diagrams consist of three unrul hypersurfaces (liquids with fold, solidus and solvus) and three ruled hypersurfaces on the borders of three-phase region (fig. 5a) [12]. T-x-y-z diagram with two eutectic solubility gaps is bounded by two T-x-y diagrams with one eutectic solubility gap, one T-x-y diagram with two binary eutectic points and one T-x-y diagrams with the continuous range of solid solution (fig. 5b). Given diagram also includes three unrul hypersurfaces and three ruled ones. Both diagrams have a complex structure of liquids and solidus with large quantity of points on contour. Therefore for both cases the liquids hypersurfaces are simulated from three fragments and solidus hypersurfaces are constructed from two parts. T-x-y-z diagrams with three-six solubility gaps don't require the additional fragmentation for their simulation and each hypersurface is described by one equation.

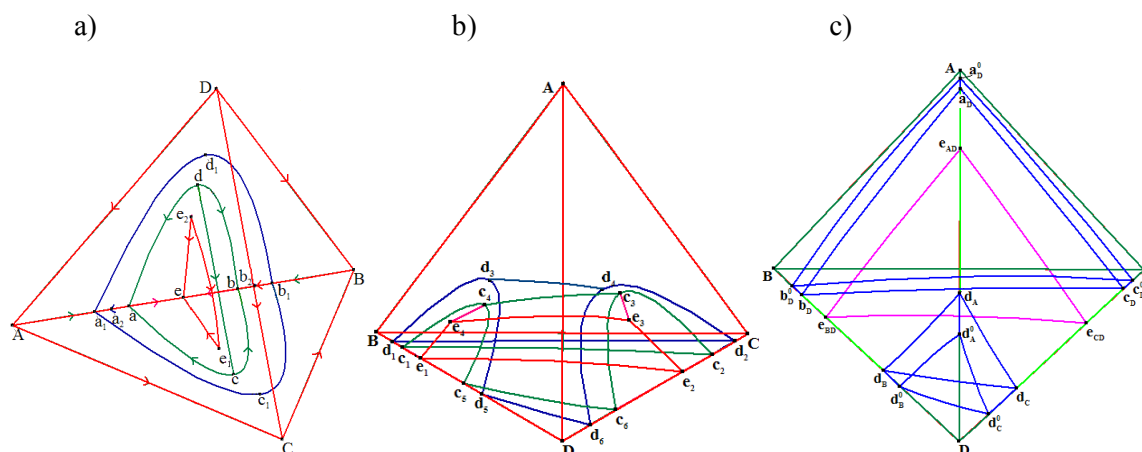


Fig. 5. T-x-y-z diagram model with one (a), two (b) and three (c) eutectic solubility gaps

Let's consider T-x-y-z diagram with two eutectic solubility gaps as an example. The directing surfaces are formed by the motion of originating line of second degree along the three directing curves, each of them passes through two or three points. The liquids hypersurface is constructed from three fragments. The hypersurface fragment joining to BC edge (fig. 6a) and bounding of surface $e_1e_2e_3e_4$ is given by the moving of originating line along the three directing surfaces $e_1e_2e_3e_4$, $a_1a_2a_3a_4$ and BC(A,C)(A,B). The part of liquids hypersurface joining to vertex D (fig. 6b) is simulated as the gliding of originating line along the directing surfaces $e_1e_2e_3e_4$, $b_1b_2b_3b_4$ and the line D(A,D). In a like manner, the hypersurface fragment joining to vertex A is constructed (fig. 6c).

The solidus hypersurface is formed from two parts. The fragment joining to side ABC (fig. 6d) is given by the shifting of originating line along the part of intersection surfaces of solidus and solvus $c_1c_2c_3c_4$ and the surfaces coinciding with tetrahedral side ABC in the projection. The fragment joining to vertex D (fig. 6e) is formed by the gliding of originating line along the other part of intersection surface of solidus and solvus $c_3c_4c_5c_6$ and line D(D,B).

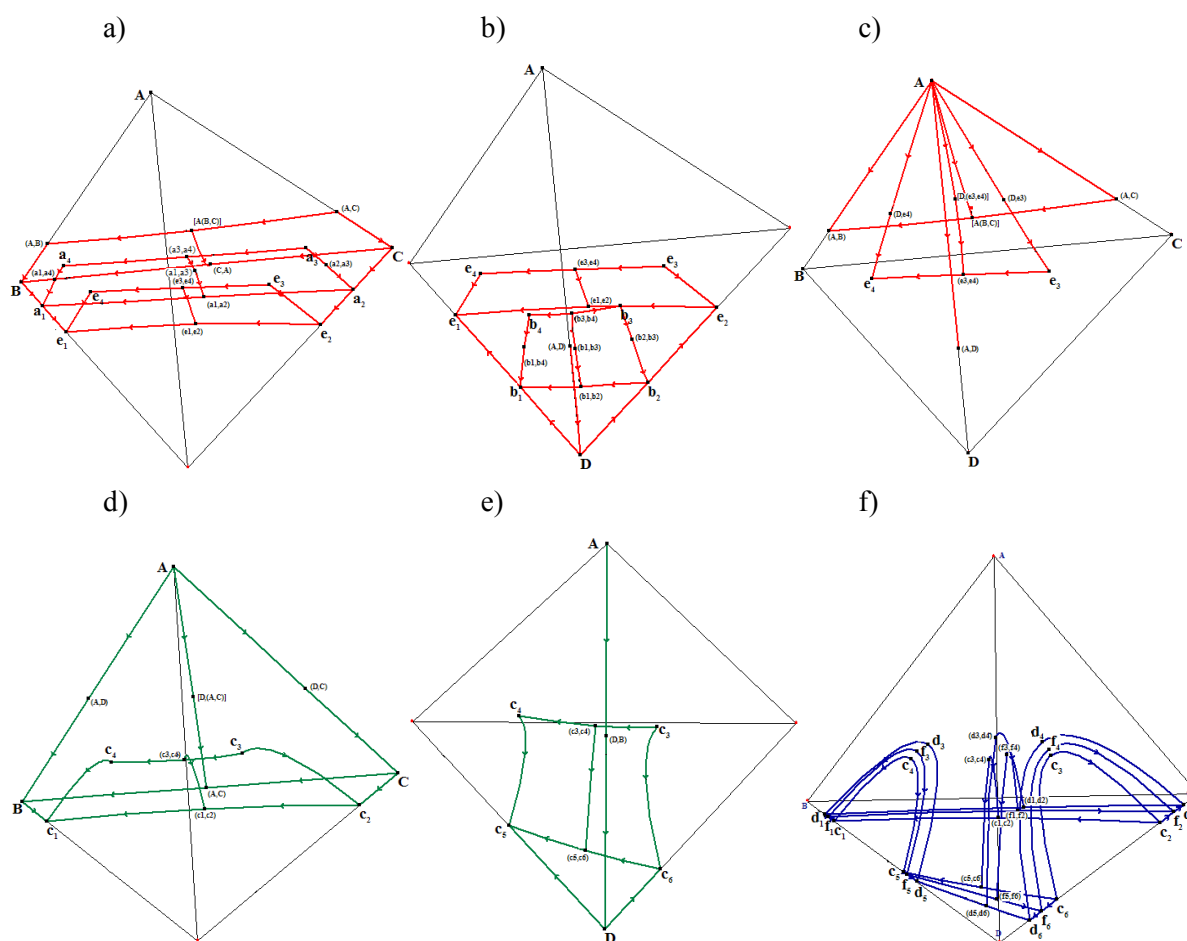


Fig. 6. The hypersurfaces of liquids (a-c), solidus (d-e) and solvus (f) fragments models)

a)

b)

c)

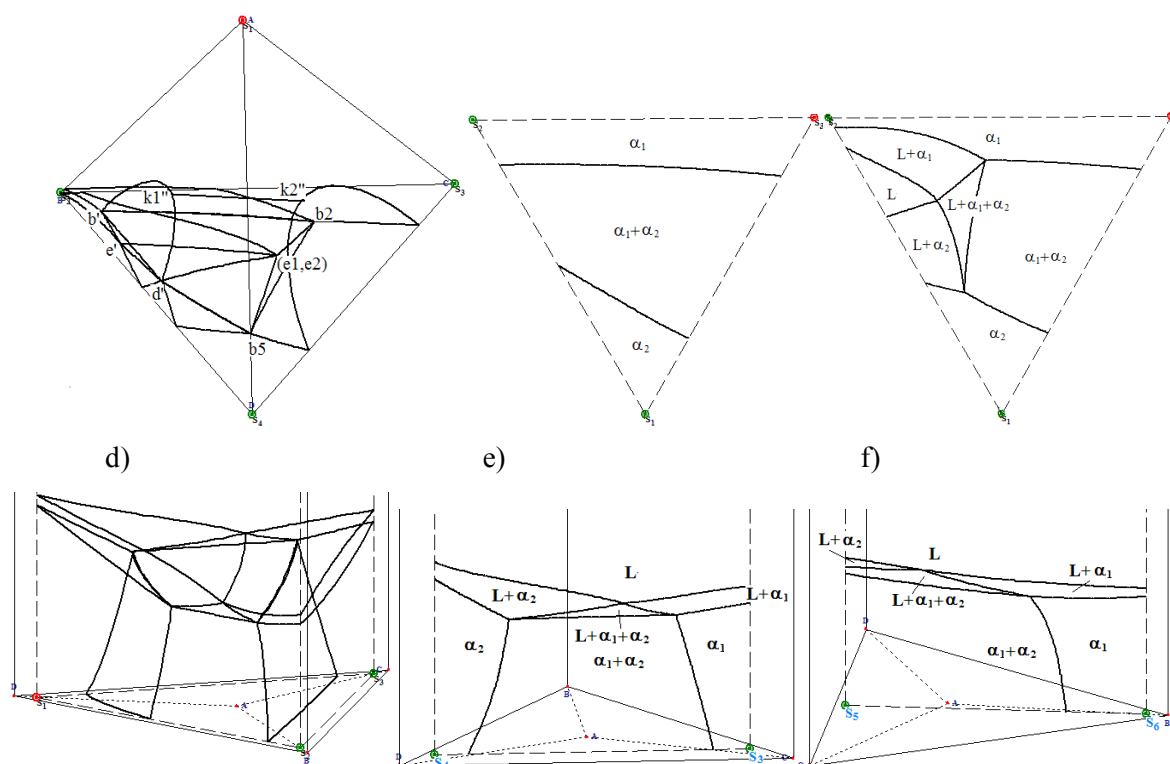


Fig. 7. The horizontal section $T_{e1} > T_{sech} > T_{e2}$ (a) and its two-dimensional sections (b-c), the vertical sections $S_1(0,1; 0; 0; 0,9)$ $S_2(0,1; 0,9; 0; 0)$ $S_3(0,1; 0; 0,9; 0)$ (d) and its two-dimensional sections $S_4(0,1; 0,1; 0; 0,8)$ (e), $S_5(0,1; 0; 0,5; 0,4)$ $S_6(0,1; 0,9; 0; 0,1)$ (f)

The solvus is described by one equation and presented as one hypersurface obtaining by the moving of originating line along the intersection surface of solidus and solvus $c_1c_2c_3c_4c_5c_6$, intersection surface of solvus and prism base $d_1d_2d_3d_4d_5d_6$ and intermediate surface $f_1f_2f_3f_4f_5f_6$ (fig. 6f).

For the obtained T-x-y-z diagram model the arbitrary three- and two-dimensional horizontal and vertical sections can be building (fig. 7).

Using the mathematical methods of phase diagrams elements descriptions at the computer software allow to simulate all geometrical structure of diagram on a basis of minimum initial information. At that the effectiveness of corresponding physics-chemical systems study is increased: the visualization of diagram geometrical model and its sections has been possible, the founding of information about the results of initial components interaction for the work content reduction of new materials creation has become available. Such software makes possible to solve the problem of heterogenous materials computer simulation.

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