Quaternary Reciprocal Systems with the Inner Diagonals: Variants of Polyhedration

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Abstract. New algorithm has been offered to divide a concentration complex of reciprocal system for the subsystems. It is based on the relations between the number of complex polyhedron vertexes and resulting number of simplexes. Method is demonstrated on the quaternary systems. It is easy realized in the software, and is very effective in the cases with inner points (compounds) and with the competition of inner diagonals.

Introduction

Usually [1] the adjacency matrix is used for the multicomponent systems polyhedration. As this process is very time-consuming, especially at many additional vertexes (new compounds) of polyhedron, special software has been elaborated [2]. Its input is an adjacency list (formed from the adjacency matrix zero elements) and its output is a list of simplexes. The program [3] defines interrelation between concentration coordinates of subsystems, formed in the initial system and given by chemical elements, and determines condition when the point belongs to the given concentration simplex or complex (at $0<X_i<1$ for all solutions of the matrix equation $Z=MX$, where matrixes $Z$ and $M$ describes the point coordinates and the subsystem vertexes concentration).

Method of A. Zykov, used in graphs theory to design the independent sub-graphs family on the base of the adjacency matrix $R$ and its list $R_1$ [4], may be applied for polyhedration too. A. Kraeva was first [5], who used it for the polyhedrons dividing (with zero elements in the adjacency list $R_1$).

So, the algorithm may be named as the ZK Algorithm (of Zykov-Kraeva).

Polyhedration by the ZK algorithm

The polyhedron with triangulated faces is presented as a non-oriented graph. Its original vertexes and the points of new compounds (on edges, faces and inside it) are numbered. Elements of the adjacency list are zero elements of the adjacency matrix. They are multiplied with regard to the absorption law. The inversion is applying to the multiplication result. And at last the simplexes list is formed. The system K, Ca, Na||NO\textsubscript{3}, Cl has two binary $D_1=$KCl-CaCl\textsubscript{2}, $D_2=$KNO\textsubscript{3}-2Ca(NO\textsubscript{3})\textsubscript{2} and a ternary $D_3=$KNO\textsubscript{3}-2Ca(NO\textsubscript{3})\textsubscript{2}-KCl [6] compounds (Fig. 1). Connections NaNO\textsubscript{3}-D\textsubscript{2}, $D_2-D_3$, KNO\textsubscript{3}-D\textsubscript{3}, Ca(NO\textsubscript{3})\textsubscript{2}-D\textsubscript{3}, KCl-D\textsubscript{3}, Ca(NO\textsubscript{3})\textsubscript{2}-D\textsubscript{1}, NaCl-Ca(NO\textsubscript{3})\textsubscript{2}, NaCl-KNO\textsubscript{3}, $D_1-D_3$, $D_1-$NaCl in bordering systems have been given \textit{a posteriori}. All points are numerated: $x_2=$KCl, $x_3=$CaCl\textsubscript{2}, $x_4=$NaCl, $x_5=$KNO\textsubscript{3}, $x_6=$Ca(NO\textsubscript{3})\textsubscript{2}, $x_7=$NaNO\textsubscript{3}, $x_8=$D\textsubscript{1}, $x_9=$D\textsubscript{2}, $x_{10}=$D\textsubscript{3}. Two pairs of lines $x_6x_7+x_6x_9$ or $x_3x_8+x_3x_{10}$ are in competition to be the inner diagonals. If to use the connections $x_6x_7$ and $x_6x_9$, then an algorithm outputs only five 3D simplexes (tetrahedrons) and six 2D simplexes (triangles). Hence, these inner diagonals do not satisfy the given triangulation of the prism faces. So, other connections are to be used: $x_3x_8=$(NaCl)(D\textsubscript{2}), $x_5x_9=$(NaCl)(D\textsubscript{3}). After multiplication according to the absorption law $(x_1+x_2+x_3+x_4+x_5+x_6+x_7+x_8+x_9)(x_{10})=(x_6+x_7)(x_9)=(x_6+x_9)=(x_3+x_4)(x_7+x_8)=(x_3+x_4)(x_7+x_8)$ and inverse of each product, the polyhedration is successfully finished by dividing the initial complex into 8 simplexes: $X_1X_2X_3X_4X_5X_6X_7X_8$.
The system Na,K||MoO₄,WO₄,F (Fig. 1) has incongruent D₁=2NaF-Na₂MoO₄, D₂=2NaF-Na₂MoO₄, D₃=Na₂MoO₄-K₂MoO₄, D₄=Na₂WO₄-K₂WO₄ and congruent D₅=KF-K₂MoO₄, D₆=KF-K₂WO₄ compounds. They form micro-complexes x₁x₂x₃x₈, x₁x₂x₉x₁₀, x₄x₅x₆x₁₀, x₄x₅x₁₁x₁₂ and x₇x₈x₉x₁₀ of solid solutions [1].

Fig. 2. To the left: 2 variants of polyhedration for a compound x₇ and competition of the diagonal x₃x₇ with the plane x₂x₄x₆ (a); common tetrahedrons x₁x₂x₃x₄, x₂x₅x₆x₇ (b); additional tetrahedrons x₃x₄x₆x₉, x₂x₄x₆x₇, if to divide by the plane x₂x₄x₆ (c); additional tetrahedrons x₂x₃x₄x₇, x₂x₃x₆x₇, x₃x₄x₆x₇, if to divide by the common diagonal x₂x₇ of 3 faces x₂x₃x₇, x₂x₄x₇, x₃x₄x₇ (d); undivided micro-complex x₃x₄x₅x₆x₇ (e). To the right: 3 variants of polyhedration for binary compounds x₇, x₈: 2 common tetrahedrons x₁x₂x₃x₈, x₂x₃x₅x₈ (a); 3 additional tetrahedrons x₁x₄x₅x₆, x₁x₅x₆x₈, x₁x₇x₈x₈, if to divide without inner diagonals (b), it is the only variant, identified by the ZK Algorithm; 4 additional tetrahedrons x₁x₄x₅x₆, x₁x₄x₅x₈, x₁x₅x⁶x₈, x₄x₅x₆x₈, x₁x₅x₇x₈, if to divide by the diagonal x₄x₈ and its faces x₁x₄x₈, x₄x₅x₈, x₄x₆x₈ (c); 4 additional tetrahedrons x₁x₄x₅x₆, x₁x₄x₅x₈, x₁x₆x₇x₈, x₅x₆x₇x₈, if to divide by the diagonal x₆x₇ and its faces x₁x₆x₇, x₃x₆x₇, x₆x₇x₈ (d).
The adjacency list after multiplication and inverse gives a tetrahedron $x_3x_6x_{11}x_{12}$, two inner planes $x_3x_6x_{10}+x_4x_5x_5$, a fragment of upper face $x_3x_7x_8$ and 4 symmetric pairs of triangles on the quadrangle faces $x_1x_2x_9+x_2x_3x_8$, $x_3x_4x_5+x_5x_6x_{10}$, $x_3x_4x_9+x_6x_7x_{10}$, $x_4x_5x_{11}+x_5x_6x_{12}$. To underline the existence of micro-complexes with solid solutions and to fulfill the dividing to the finish, it is necessary to use some virtual diagonals not only on corresponding faces (or their fragments), but on the diagonal plane $D_1D_2D_3D_4D_5=x_3x_7x_{10}x_{12}$ too. Then elements $r_{1,8}$, $r_{1,10}$, $r_{2,7}$, $r_{2,9}$, $r_{4,10}$, $r_{4,12}$, $r_{5,9}$, $r_{5,11}$, $r_{7,10}$, $r_{8,9}$ become equal to 1 (they are deleted from $R_j$) and the multiplication $(x_7+x_3x_4x_5x_6x_{11}x_{12})^\text{ops} = (x_2+x_3x_4x_5x_6x_{11}x_{12})^\text{ops} = (x_6+x_3x_4x_5x_6x_{11}x_{12})^\text{ops}$.

**Algorithm in the system with two binary compounds**

The ZK Algorithm in the system with a binary compound $x_7$ on the plane $D_2$ and to describe it by the adjacency matrix and to know the only variant without diagonal.

**Algorithm limitations**

Algorithm can not divide the polyhedron with inner points [2, 6, 7] and with competition of inner diagonals and planes. For instance, two variants of polyhedronization in the quaternary reciprocal system with a binary compound $x_7$ in the ternary system $x_4x_5x_6$ (Fig. 2, left) are possible because of competition between the diagonal $x_3x_7$ and the plane $x_2x_4x_6$. Polyhedronization gives two tetrahedrons in both cases and two or three additional tetrahedrons. But the ZK Algorithm fulfills the only as a result a tetrahedron $x_3x_6x_{11}x_{12}$, one 6-vertex $x_4x_5x_6x_{10}$ micro-complex and three 5-vertex $x_3x_4x_5x_6x_{10}$ micro-complexes of solid solutions.

**Topological rules for A.B.C||X,Y polyhedrons**

If to present a tringular prism of the quaternary reciprocal system $A,B||X,Y,Z$ (or $A,B,C||X,Y$) as a graph and to describe it by the adjacency matrix, then for $V$ vertices of the graph and $J$ its joinings (connections) their numbers are equal to: $V=V_0+V_E+V_f+V_I$ and $J=J_0+J_E+J_I$.

**New algorithm of polyhedron**

Because of ZK Algorithm shortcomings, the New Algorithm has been elaborated. In contrast to the ZK Algorithm the new one works with “1” elements of the adjacency matrix. It consists of three steps: 1) All connections $x_ix_j$, including all possible inner diagonals (lines, connecting every binary compound of both triangular faces of the prism with opposite vertexes), are written; 2) All possible planes $x_ix_jx_k$ of three types are formed: $S_I$ planes on faces, $S_I^*$ inner planes without inner diagonals on their sides and $S_I^{**}$ inner planes, connected with possible inner diagonals. The last type of planes ($S_I^{**}$) is analyzed in accordance to formulas (2), which estimate all probable variants of polyhedron.
and confirm only those combinations of $S_i^{**}$ planes, that produce together with $S_F$ and $S_i^*$ all possible tetrahedrons; 3) All $S_F$, $S_i^*$ and selected at the second step planes $S_i^{**}$ form tetrahedrons of two types, with and without the inner diagonals. The New Algorithm put out all possible variants of polyhedration in competition of inner diagonal elements: lines and planes. So, the last step is to confirm experimentally which of inner diagonals and planes must participate in polyhedration. It permits to find tetrahedrons, which the ZK Algorithm doesn’t identify.

**Problems with the polyhedration of K,Li,Ba||F,WO$_4$ system**

Six polyhedron vertexes and 4 compounds [8] are enumerated: $x_1$=KF, $x_2$=LiF, $x_3$=BaF$_2$, $x_4$=K$_2$WO$_4$, $x_5$=Li$_2$WO$_4$, $x_6$=BaWO$_4$, $x_7$=LiBaF$_3$SO$_4$, $x_8$=K$_3$FWO$_4$, $x_9$=D$_2$=LiKWO$_4$, $x_{10}$=D$_3$=K$_2$Ba(WO$_4$)$_2$ (Fig. 3). As any binary compound on the side of a ternary system (excluding the common edges of two reciprocal systems) should be connected with opposite vertexes of the prism, then the compound $x_7$=LiBaF$_3$SO$_4$ may be connected with vertexes $x_4$, $x_8$, $x_9$, $x_{10}$, and $x_9$ – with $x_3$, $x_7$, and $x_{10}$ - with $x_2$, $x_7$ (Fig. 3). Inner diagonals must not be intersected inside the prism, so it is necessary to enquire all possible variants of their intersections (analytically, by the resolving of corresponding equations) and then to analyze them. Results of types “inner cross-section exists” (“+”) or “it is absent” (“−”) are in the Table 1. (Obviously, lines $x_4x_7$, $x_3x_8$, $x_2x_9$, $x_7x_{10}$ have a common point $x_7$, lines $x_2x_{10}$ and $x_7x_{10}$ – common point $x_{10}$, lines $x_3x_9$ and $x_7x_9$ – common point $x_9$, but the inner intersections on the faces or inside the prism are prohibited).

![Fig. 3. Triangulated faces of prism K,Li,Ba||F,WO$_4$ and 3 variants of its tetrahedration by alternative inner diagonals: $x_2x_4x_9x_{10}$, $x_2x_3x_8x_{10}$, $x_2x_4x_7x_{10}$, $x_2x_3x_7x_{10}$, $x_2x_6x_9x_{10}$, $x_2x_6x_7x_{10}$, $x_3x_6x_7x_{10}$, $x_2x_3x_6x_{10}$ by $x_2x_{10}$+$x_3x_{10}$ (a); $x_3x_4x_9x_{10}$, $x_3x_4x_7x_{10}$, $x_3x_4x_8x_{10}$, $x_3x_4x_7x_{10}$, $x_3x_4x_6x_{10}$ by $x_3x_9$+$x_4x_10$ (b); $x_2x_4x_9x_{10}$, $x_2x_4x_7x_{10}$, $x_2x_4x_8x_{10}$, $x_2x_4x_7x_{10}$, $x_2x_4x_6x_{10}$ by $x_7x_9$+$x_7x_{10}$ (c).]
Table 1. Variants of possible cross-sections for inner diagonals (Fig. 3)

<table>
<thead>
<tr>
<th>$J_f$</th>
<th>Diagonals</th>
<th>Inner planes</th>
<th>Tetrahedrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-</td>
<td>$x_3x_9$</td>
<td>1&lt;6</td>
</tr>
<tr>
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<td>$x_3x_8$</td>
<td>$x_3x_8+x_3x_9$, $x_3x_8$, $x_3x_9$</td>
<td>1+3=4&lt;8</td>
</tr>
<tr>
<td>1</td>
<td>$x_3x_{10}$</td>
<td>$x_3x_9+y+x_3x_{10}$, $x_3x_{10}$</td>
<td>1+2=3&lt;8</td>
</tr>
<tr>
<td>2</td>
<td>$x_3x_8+x_3x_{10}$</td>
<td>$x_3x_8+x_3x_{10}$, $x_3x_{10}$, $x_3x_8+x_3x_{10}$, $x_3x_8$</td>
<td>1+3+2=6&lt;10</td>
</tr>
<tr>
<td>2</td>
<td>$x_3x_{10}+x_3x_{10}$</td>
<td>$x_3x_{10}+x_3x_{10}$, $x_3x_{10}$, $x_3x_{10}+x_3x_{10}$, $x_3x_{10}$</td>
<td>1+4+2=7&lt;10</td>
</tr>
<tr>
<td>2</td>
<td>$x_3x_9+x_3x_{10}$</td>
<td>$x_3x_8+x_3x_{10}$, $x_3x_{10}$, $x_3x_9+x_3x_{10}$, $x_3x_8$</td>
<td>1+4+3=8&lt;10</td>
</tr>
<tr>
<td>3</td>
<td>$x_3x_{10}+x_3x_9+x_3x_{10}$</td>
<td>$x_3x_{10}+x_3x_9+x_3x_{10}$, $x_3x_{10}$, $x_3x_9+x_3x_{10}$, $x_3x_9$</td>
<td>1+4+3+2=10&lt;12</td>
</tr>
<tr>
<td>3</td>
<td>$x_3x_9$</td>
<td>$x_3x_8+x_3x_{10}$, $x_3x_9$</td>
<td>1+4+3+3=11&lt;12</td>
</tr>
<tr>
<td>4</td>
<td>$x_3x_{10}+x_3x_{10}$</td>
<td>$x_3x_{10}+x_3x_{10}$, $x_3x_{10}$, $x_3x_{10}+x_3x_{10}$, $x_3x_{10}$</td>
<td>1+4+4+5+3=14</td>
</tr>
<tr>
<td>4</td>
<td>$x_3x_9+x_3x_{10}$</td>
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<td>1+4+4+5+3+3=16</td>
</tr>
<tr>
<td>4</td>
<td>$x_3x_9$</td>
<td>$x_3x_9+x_3x_{10}$, $x_3x_9$</td>
<td>1+4+4+5+3+3=16</td>
</tr>
</tbody>
</table>

As lines $x_3x_7$ and $x_7x_9$ have no inner intersections, they are the doubtless diagonals. The line $x_3x_{10}$ is intersected with $x_3x_9$ and $x_7x_9$. Alternative to $x_3x_{10}$ diagonal, a $x_3x_9$ one can coexist only with the diagonal $x_7x_9$. (They coexist with $x_4x_7+x_7x_8$). So, it is necessary to testify the variants with alternative diagonals $x_3x_{10}$ and $x_3x_9$: $x_3x_{10}+x_3x_7+x_8x_7+x_7x_9$, $x_3x_9+x_4x_7+x_7x_8+x_9x_9$. Third variant has no both alternative diagonals $x_3x_{10}$ and $x_3x_9$: $x_4x_7+x_7x_9+x_7x_9+x_7x_{10}$.

Table 2. Enquiring of possible polyhedrons variants according to formulas (2). Variants at $J_f>4$ are impossible because of $x_3x_{10}$ intersection with $x_3x_9$ and $x_7x_9$ - with $x_3x_{10}$

As the system has $P_2=4$ binary compounds ($x_7$, $x_9$, $x_{10}$ are on the upper triangular face of the prism, $x_8$ is on its vertical edge). then, according to formulas (2): $J_f=9+P_2=13$, $J_f=3+2P_2=11$, $S_f=8+2P_2=16$, numbers of inner diagonals $J_f(x_3x_{10}, x_3x_9, x_3x_8, x_7x_9$ and $x_7x_{10} )$ may vary from 0 to 6, inner planes $S_f=2+P_2+2J_f$ from 6 at $J_f=0$ to 18 at $J_f=6$, 3D simplexes $T=3+P_2+J_f$ from 7 at $J_f=0$ to 13 at $J_f=6$.

**Step 1:** All $J_f+J_f+J_f=13+11+6=30$ connections are written:
- $J_f=6$ possible inner diagonals $x_2x_{10}$, $x_3x_9$, $x_4x_7$, $x_7x_8$, $x_7x_9$, $x_7x_{10}$;
- $J_f=13$ edges $x_1x_2$, $x_1x_3$, $x_1x_9$, $x_2x_5$, $x_2x_7$, $x_2x_9$, $x_3x_7$, $x_4x_8$, $x_4x_9$, $x_4x_{10}$, $x_5x_6$, $x_5x_9$, $x_6x_{10}$;
- $J_f=11$ diagonals on faces $x_1x_7$, $x_1x_9$, $x_2x_6$, $x_2x_9$, $x_3x_4$, $x_3x_8$, $x_4x_8$, $x_4x_{10}$, $x_5x_7$, $x_6x_9$, $x_9x_{10}$.

**Step 2:** All permitted planes (37 2D simplexes) are formed from 30 connections:
- $S_f=16$ planes on faces $(x_1x_2x_7, x_1x_3x_7)$, $(x_2x_4x_{10}, x_3x_4x_9, x_5x_6x_9, x_7x_9)$, $(x_1x_3x_8, x_2x_4x_8, x_3x_4x_9, x_2x_3x_9, x_2x_4x_7)$, $(x_2x_3x_8, x_2x_3x_9, x_2x_3x_7)$;
- $S_f^*=1$ plane $x_3x_9y$ inside the prism without inner diagonals;
- $S_f^{**}=20$ planes with six different inner diagonals: $x_2x_{10}$ ($x_2x_4x_{10}$, $x_2x_6x_{10}$, $x_2x_7x_{10}$, $x_2x_9x_{10}$), $x_3x_9$ ($x_1x_4x_9$, $x_1x_3x_9$, $x_1x_3x_9$, $x_3x_3x_9$, $x_3x_3x_9$), $x_4x_7$ ($x_2x_4x_7$, $x_3x_4x_7$, $x_4x_7x_8$, $x_4x_7x_9$, $x_4x_7x_{10}$), $x_5x_8$ ($x_1x_7x_8$, $x_2x_7x_8$, $x_3x_7x_8$, $x_7x_9$) ($x_2x_7x_9$, $x_6x_7x_9$, $x_7x_9x_{10}$), $x_7x_{10}$ ($x_3x_7x_{10}$, $x_6x_7x_{10}$).
Step 3: variants of polyhedration with 4 inner diagonals can be realized.

The inner plane $x_{2}x_{6}x_{9}$ and $S_{I}=16$ planes on faces together with $S_{E}=2+P_{E}+2J=14$ inner planes at $J=4$ diagonals produce $T=3+P_{E}+J=11$ ($P_{E}=J=4$) tetrahedrons (Fig. 6): a tetrahedron $x_{2}x_{6}x_{9}$ - without inner diagonals;

- 4 tetrahedrons $x_{1}x_{2}x_{7}x_{8}$, $x_{1}x_{3}x_{7}x_{8}$, $x_{2}x_{4}x_{7}x_{8}$, $x_{3}x_{4}x_{7}x_{8}$, produced by diagonals $x_{4}x_{7}+x_{7}x_{8}$;

- 6 tetrahedrons (on dependence of a choice of second pair of diagonals).

Conclusions

1) Software, based by the ZK Algorithm [4, 5], had been elaborated. It consists of four steps: - to represent n-component system as a graph, - to record the adjacency list with the adjacency matrix zero elements, - to multiply the adjacency list elements accounting the absorption law, - to fulfill inversion; - to sort out all possible polyhedration variants and to drop the ones, non-real geometrically or non-supported by experiment. Systems with solid solutions requires additional virtual diagonals. Polyhedration with inner isolated points is fulfilled in two stages: without inner points at first and with inner points in micro-complexes.

2) Interrelations between the number of inner diagonal planes and simplexes on the one hand and non-zero elements of the adjacency matrix on the other hand had been got. They are very useful for the original data and program output verification and give a possibility to estimate the polyhedration result a priory.

3) The New Algorithm has been elaborated. It may be applied for polyhedration of quaternary and more complex multicomponent systems (including the reciprocal ones) and it is able to identify all variants of polyhedration, including situations, when the ZK Algorithm can not “recognize” some simplexes.

4) Topological Rules embrace interrelations between all geometrical elements of polyhedron, including its binary, ternary subsystems and binary, ternary, quaternary compounds (systems with quaternary compounds were not yet analyzed).

References


