Separation-Mixing as a Model of Composition Evolution of any Nature

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ABSTRACT

Model of separation-mixing is applicable when studying the compositional evolution of systems of different nature, from physicochemical to the social ones. To display the processes, ***RHAT*** information language-method is proposed; it takes into account at the same point on the chart an indefinitely wide variation of components and their quantity. The possibilities of the model application are showed.

Keywords: Composition, Heuristics, Method ***RHAT***, Mixing, Separation, Purity, Separation Entropy,

1. INTRODUCTION

There are concepts that guide thinking to the general view on what is happening in the world. Herbert Spencer distinguished differentiation and integration as two fundamental processes of complex systems evolution in nature, technology, and society. In particular, in the evolution of systems completely different in material embodiment, there is a similarity in their composition change. A person can directly observe only the processes taking place in mobile environments and during their manifestations observed for the period of life: seasonal and annual changes in ecosystem, composition of waters, rivers. The processes taking place in the Earth interior are not observable and are slow. Information about them is obtained indirectly by studying their tracks - spatial distributions of compositions of rocks and their component parts – minerals, inclusions in them, as well as intergranular substance [1]. Geology as a science with a great practical output, with a specific set of macroscopic characteristics of the study object [2], is a good model for heuristically important analogies with other branches of knowledge. Another model object – crystal, the formation processes of which are deeply developed theoretically [3] can be used as a model for the study of a wide variety of separation processes, in which the great role of a chance is combined with the strictness of laws of physics and physical chemistry. In 1971, paper [4] was published, which presented the method of compositions encoding designed for describing and classification of discrete distributions of any nature. The possibility to represent a system as a discrete series of event names with ranking by decrease of their probabilities should be common to them. The method also enables to study the processes of compositions change, which makes it possible to use it for reflecting the separation-mixing processes.

The paper aims to describe the processes of separation and mixing as model ones to study the evolution of compositions of different nature, as well as the information language for their representation, *RHAT* method.

2. MODEL OF SEPARATION-MIXING

Separation is the process of formation from a system of two or more systems differing in composition, which can be written as A→B+C+…. Examples: crystallization from solutions, various types of separation using various fields and sieves, centrifuges, distillation, formation of mineral deposits, in chemistry - reactions of substances decomposition. It is trivial, but the existence of different "elements" is essential in the system, by which we mean - the minimum "parts-particles" of components. Mixing is the process of combining of systems different in composition with composition homogenization in their common space. Designation: A+B+C+...=D. Examples: various kinds of dissolution, waste disposal into the environment, soil fertilizing, preparation of construction, pharmaceutical, food mixes, in chemistry reactions of substances combination occur as a result of mixing. Successive mixing and separation is a common in geology process of replacement (A+B→C+D); its result coincides with that of separation. In this case, some of its products, being more mobile, can disappear from view creating effects remote in space and time.

The system arising as a result of mixing has an average composition in all components between the compositions of the original systems. Maximum contents decrease, minimum increase. In contrast to mixing, as a result of separation some elements get increased contents compared with the original system, the others – decreased ones. That is, ***only separation causes growth and fall of the component contents*** in the resulting system compared to the original ones. In engineering processes, separation is enrichment – ***increasing of major component contents***, and ***purification*** – ***decreasing of minor, small contents, "admixtures"***. In contrast to laboratory, where the act of mixing occurs, one may say, in a single step, and processes of composition change are stretched in time and space in nature. They leave their traces in the form of a volumetric cloud of more or less smoothly varying compositions, in which a geologist looks for the directions of maximum variability in order to understand where the solution - the originator of changes - came from, where is the maximum concentration of the substance of interest.

General condition for the separation and mixing processes is the presence of translational mobility at particles of all or some components of the original systems. Therefore, they can pass only at not too low internal energies. As the temperature increases, bonds are torn and the substances pass into liquid and gaseous state, which leads to the predominance of mixing processes. In closed systems, which are in an impermeable for the substance container, energy increase leads to the prevalence of trend to mixing, up to the inclusion of its walls in this process. As the gases temperature decreases, the reverse processes take place: condensation (water droplets in the air), crystallization (formation of snowflakes, crystallization in magma). That is, the existence of separation or mixing depends on the total energy background of the system. Curve of substances solubility-miscibility is the border between the separation and mixing and, at the same time, between the fields of "content-temperature" pairs. At "too low" energies, translational mobility is missing - the system is "frozen".

Differences in elements mobility can be generally (but with some care) regarded as a driving force of separation. Such differences are due to the temperature difference in gas and liquid that are in a closed system, where in a higher temperature area more mobile system elements are accumulated (Soret effect), or when using filters, or slowdown and fixing of substance on the growing crystal surface. Crystallization is a demonstrative example of separation [5,6] of gas or liquid mixtures, solutions, and simultaneous self-organization, to which the conference was dedicated in 1961 [7]. ***Crystal is a result of a flow of random events***, namely the selection acts of individual atoms-molecules-radicals with respect to their bonding energies to this place on the crystal surface. These selections are made for each particle until it is overlapped by the following particles, also undergoing these selections [8]. And these selections take place with errors that accompany the construction of what will probably be always seen as the acme of perfection - in nature, technology, and in our minds. Growing crystal perhaps is the best example of self-organization of matter. In this case, changes in the "growth pyramids" composition of different faces of a grown crystal bear the record on its formation history. The question on the driving force of mixing is more difficult. In the simplest case, for gases, the driving force of mixing is the desire to pass into a more probable and disordered state. Generally, miscibility - ability to a more uniform distribution of different parts-particles in the volume grows with energy increase (explosions, tornadoes, tsunamis etc.). However, "in case of a moderate" energy background, when the temperature decreases the system will sooner or later come first to equilibrium with the liquid or crystalline phase, and then to separation.

In addition to the polarity of the considered processes ***results***, there is another polarity. This is the polarity of separation and mixing ***rates***. Separation processes rates are regularly lower than those of mixing processes. The first direct measurements of rates of crystal growth and dissolution under equal overheating-overcooling have shown this. [9]. Probably, it is well known that in general all processes associated with the need to distinguish, to separate, to organize have lower rates than the processes of mixing, disordering. It is known in the same context that the lower the difference between component particles, and the smaller they are the slower and less efficient is the selection, sorting.

When studying composition evolution, the determination of its direction and path length estimation are hindered by fragmented character and often incompleteness of materials. In addition, the following is substantial: a) uncertainty of selecting the "main" parameter, as the "main" component at the early stages of the process can become absolutely insignificant at the late ones; b) opposite direction of changes of various parameters, which is caused by composition normalizing to a unity (or 100%); c) absence of a time-constant direction of changes in individual components, in particular, because of the imposition on the "main" process of the subsequent ones or preservation of traces of previous.

Such difficulties could be overcome with the help of using the integral characteristics of process, specifically focused on the representation of separation-mixing processes.

Despite the abundance of well-known to the author descriptions of separation in engineering processes, variants for differentiation in nature, destructive consequences of separation in social systems based on religious, national, property and other features, works on "separation of powers", it should be admitted that he was unable to find papers on the general theory of separation. However, on the theory of mixing - too. Applied to the geological problems, the considered processes are described in [5].

Speaking of substance circulation in nature, one can say the following: any mixture will sooner or later undergo separation – dissociation; any separation products sooner or later will participate in mixing. Any mixing-association is temporary, any separation – dissociation in nature is for ever.

Such circulation exists on the surface and in the interior of the Earth, and under the leading influence of gravity it caused the division of its whole material into the lithosphere, hydrosphere, and atmosphere.

3. *H, A, T* INTEGRAL CHARACTERISTICS OF COMPOSITIONS

To display the separation and mixing processes, we use a combination of C. Shannon information entropy ***H*** as a characteristic of complexity and anentropy ***A*** [4,10,11,12] as a characteristic of composition purity as a basis. The use of the Shannon entropy is substantiated by two circumstances. First, mixing entropy existing in thermodynamics is different from the Shannon only by factor, the gas constant. Second, [13] proved two theorems on the entropy change during separation and mixing. When two systems are separated, entropy of at least one of the resulting systems is lower than entropy of the original one. When two systems differing in composition are mixed, entropy of the resulting system is greater than that of at least one of the original systems. These theorems give a statistically significant substantiation for entropy decrease during separation and its increase during mixing. There is no such evidence for anentropy, however the commonness of inverse relationship between anentropy and entropy does not prevent their joint utilization in diagrams.

C. Shannon information entropy $\boldsymbol{H}= - \Sigma \boldsymbol{p}_i * \lg \boldsymbol{p}_i$ as a measure of uncertainty – complexity of the next event prediction. With regard to intuitively understood concept of composition complexity, there are two polar distributions of content. 1) Uniform: when there are many components and all components are in equal proportion, complexity is high and is $\lg \boldsymbol{n}$. 2) Extremely uneven: when a system has only one component, complexity is zero. Extremely high complexity and extremely low purity correspond to the first case. Extremely low complexity and extreme purity, to the second one. Let us immediately note that the latter is not achievable for real chemical systems either practically, according to the principle of chemical elements ubiquity [14] or in theory, according to [15]. This should be considered a very common feature of multicomponent systems.

Apparently, entropy was for the first time used in geology [16]. Subsequently, it has become widely used in various fields of knowledge, but for a very short time in geology. The fact is that contributions to entropy [$-\boldsymbol{p}_i * \lg \boldsymbol{p}_i$] after the maximum at $\boldsymbol{p} = 0.368$ drop sharply with $\boldsymbol{p}_i$ decrease. Therefore, with $\boldsymbol{p}$ decrease its value comes down, that is the contents of small components, more valuable than the common ones, almost cease to influence $\boldsymbol{H}$ value. Moreover, the compositions that slightly differ in large but significantly different in small components become indistinguishable. Thus, rocks – shales are indistinguishable by $\boldsymbol{H}$ from minerals – some micas. This led to the search and introducing of an additional value, which would take into account small ones, and to the greater extent the smaller the content value. That is, the task was to balance the significance of large and small. The fact is that information about the major components is usually enough for identification of the object name, however for tracing the history, construction of genetic models information about the secondary, and even the smallest components is required. Their list and their concentrations bear the record on the ultimate pages of the formation history of the system being studied now.

In addition to the entropy, to account for the smallness of small components, characterization of composition purity anentropy $\boldsymbol{A} = - 1/\boldsymbol{n}(\Sigma \lg \boldsymbol{p}_i) - \lg \boldsymbol{n}$ was introduced [4,10,11,12]. Note that here $\lg \boldsymbol{p}_i$ is the component contribution to anentropy value, at the same time, it is the first derivative of $\boldsymbol{p}_i * \lg \boldsymbol{p}_i$ with respect to $\boldsymbol{p}$. That is $\boldsymbol{H}$ and $\boldsymbol{A}$ are mathematically linked together. Minimum A = 0 if all components are in equal proportions, that is when entropy is maximum. Anentropy is interpreted as entropy of separation [12]. Below one can find the diagram (Fig.1) described in detail in [12], with some changes. The diagram shows outlines of the field, inside which there are the trajectories of all processes that can occur with compositions that have ten components and content intervals from 0.99955 to 0.00005 ($\Sigma \boldsymbol{p}_i = 1$). Along the axes, directions of the trajectories during separation and mixing are showed, and inside, illustrations to formulations of Yu. Shurubor theorems.

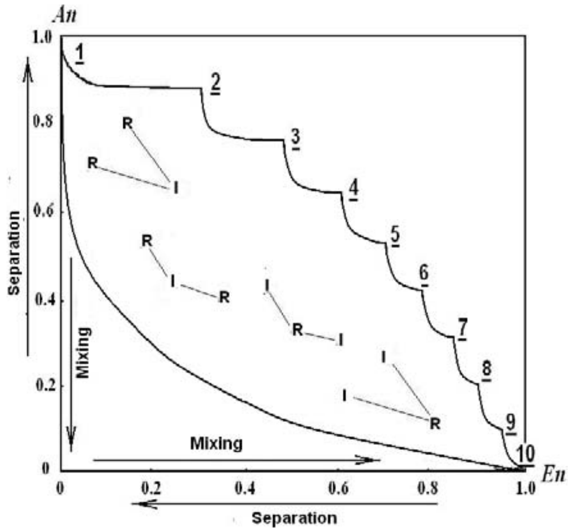

Fig.1 ***EnAn*** entropy diagram. Main directions of mixing and separation processes, as well as positions of the original [I] and resulting (R} systems are shown.

When working with especially pure substances, anentropy is insufficiently to changes in composition. Therefore, "tolerance" or "sterility" $\boldsymbol{T}$ was introduced. In the same notation $\boldsymbol{T} = \lg[1/\boldsymbol{n}\Sigma(1/\boldsymbol{p}_i)]$ [2]. In terms of information theory, $\boldsymbol{T}$ can be interpreted as logarithm of the Component contribution in $\boldsymbol{T}$ is the second derivative with respect to $\boldsymbol{p}$ of the contribution to entropy, and the first derivative of the contribution to anentropy. ***HT*** diagram is shown in Fig.2 ***average signal waiting time for their uniform arrival***.

Dependence of contribution to $\boldsymbol{H,A,T}$ on $\boldsymbol{p}$ is given in a diagram in [11].

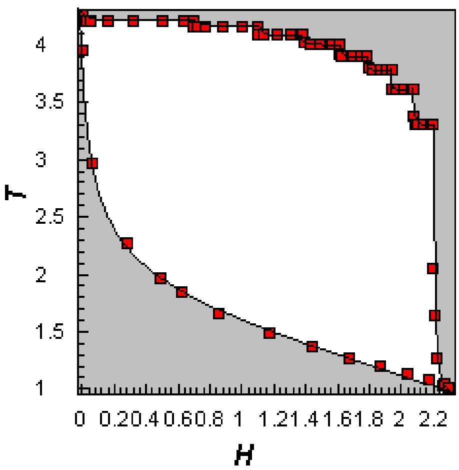

Fig. 2. Entropy-tolerance diagram. Gray - area prohibited for compositions with components content below 0.00005.

HA and ***HT*** diagrams are polar. The capability of substances to mixing (to solubility) increases with temperature growth, which usually causes ***H*** increase and ***A*** decrease of composition. ***H*** and ***A*** of separation products are associated with process intensity and noise level [16]. During crystallization, intensity increases: 1) when the system deviation from equilibrium, which determines the rate of crystallization, grows; 2) when the medium complexity grows; 3) when the temperature grows. Temperature is a "centaur". It prevents the particles ordering on the crystal surface, showing itself as noise, and conditions the required mobility of a particle when it chooses the "right" place and position [8].

4. “COMPLETENESS” OF AN OBJECT COMPOSITION

Representation integrity of a complex system composition has specific requirements to the information completeness on the quantitative relationship between its constituent parts [10]. This is due to the fact that complete and accurate information on the systems composition is usually unattainable, and all three quantitative characteristics depend on the number of components. To compare the results of ***H***,***A***,***T*** calculations, "complete" analyses are required, that is those in which all essential components for the chosen ***analysis detail n*** are present. When distinguishing components for ***HA*** calculation, ***rank formulas R*** are used, ***component sequences by content decrease***. (Analyses in the sampling should be at least no shorter than ***n*** value.) For ***n*** values of contents ***H***,***A***,***T*** are calculated. Components with numbers greater than ***n*** are ignored, they are excessive, however their quantity is a qualitative assessment of the reliability of selection of ***all n main*** components of composition. It is clear that the lists of components in such standardized analyses may not be the same (this is one of difficulties in the method development). After adjusting the rank formula, compositions are normalized to the sum of the components remaining in it. It should be borne in mind that the smaller ***n***, the less information on compositions is taken into account, it has a more general character, and vice versa. The degree of points distinctiveness in the diagram with ***n*** increase usually grows sharply at first, then slows down, so one can ***choose the optimal detail level*** for different data sets.

5. HEURISTICITY OF THE MODEL REFLECTED IN THE ENTROPY DIAGRAMS

Composition change is in principle continuous and should be displayed in the diagram by lines. The smaller the points scatter along the mean trajectory of system evolution in the diagram, the more clearly expressed the process in nature and in the diagram. Data on compositions evolution are almost always fragmentary. In addition, their sequence in the historical sciences is often poorly defined. Diagrams enable to find the most probable trajectories of the processes, to assess the length of their way and pay attention to the anomalous points. Processes of composition change of two types are the ruling ones in nature. They cause: 1) an increase of differences between the component values, and 2) a decrease of differences. With the growth of differences, ***H*** decreases, ***A*** increases. With the reduction of differences, ***H*** increases, ***A*** decreases. Other directions of trajectories correspond to the transient processes between the considered ones. In one-way processes - monotonous changes of component contents, the transition from ***H*** increase and ***A*** reduction to ***H*** decrease and ***A*** growth, as shown by numerous observations, is possible. The transition from ***H*** decrease to its increase (at the corresponding ***A*** changes) speaks for a disturbance of the process monotonicity. Several representations of various one-way process in ***HA*** diagrams are given in [12]. An example of a sharp change in the process direction in one geological object - rare earth pegmatites is given in [18]. The first stage of pegmatites development, "barren" igneous corresponds to the typical separation with complexity reduction and purity increase. At this time, gravitational settling of heavier minerals with lighter fluid separation and its crystallization as coarse-crystalline formation - "pegmatite" with decreased ***H*** and high ***A*** takes place in magma. The second stage - high-temperature aqueous solutions flowed into the cracks and pores of rock – mixing took place (***H*** growth and ***A*** decrease). Solutions reacted with pegmatite substance and deposited new substances, i.e. secondary separation took place. After depositing substances, solutions left the changed rock volume. Geologist handles with enriched in "ore" components (in this case, lithium minerals) one part of the twice separated system. Using ***H***,***A*** values enabled to reveal a system of sphalerite (ZnS) occurrences and the epicenter of ore-forming solutions source in the Northern Urals [19]. In the epicenter, sphalerite purity was minimal and increased with the distance from it along the system of faults to more than 300 km in one direction and 60 km in the other; zone width in the epicenter area of about 50 km.

Diagrams provide opportunities of reflecting composition changes in complex hierarchically structured systems, such as igneous rocks. Thus, the diagrams can combine the evolutionary trends of: a) chemical compositions of rocks [2,12], b) mineral compositions of the same rocks, c) chemical compositions of minerals building them up, g) crystal chemical characteristics of minerals [20]. The impossibility of such combinations for visual perception in the traditional forms of the actual material representation limits both the possibilities of conceptual interpretation of complex systems development and fantasy. Heuristicity of the separation-mixing model occurs when only one branch of the separation products change is easily accessible for learning during the separation process. This situation focuses on the search for other branches, possibly more valuable. An example of separation of a general group of organic substance (cellulose, lignin, proteins etc.) into gas, oil and coal [21]. Oil coming to refining is itself a complex mixture of solid, liquid, and gas substances and is subject to separation. As a result of a large number of processing separation methods, an indefinitely wide range of substances is produced. A few examples of curves obtained in the theoretical mixing of compositions of complex systems are presented in [12]. The trajectories of compositions development in a series of igneous rocks from gabbro to granite and of sand compositions are given there as well. Trajectories are quite similar as in both cases they reflect the separation processes. Physical and chemical processes during these composition changes are dramatically different.

Analogs of the separation-mixing model go far beyond thermodynamics, up to ecology, sociology, linguistics, where mixing and/or separation terms are used at a half-intuitive level, without quantitative estimates.

The simplest social-psychological analog of situation with the Soret effect - concentration in areas of military conflicts, in high-risk areas, of more energetic, courageous people, with adventurous temperament - and there is an increase of national and confessional compositions entropy.

There is a principle of optimal diversity addressed in various fields of knowledge. One way to implement it is the breakdown of complex systems with formation of simpler ones, the other way is the development of simple systems with their complication. Ethnic and religious mixing taking place in many countries could be compared in ***HA***, ***HT*** diagrams. After reaching the "supersaturation" new phases are formed, which is marked by the dissipation of states. Social activity – an equivalent of temperature - a comfortable life exists away from power poles.

Liquidation of a wide gap between the need for knowledge on the contents of light elements, elements of life and weak in this regard possibilities of the modern analytical framework - should lead to a new stage in development of knowledge about the Earth and the Life on it.

Human actions on the planet from substance concentrates mining to road traveling involve the predominance of diminishing, dispersion, and therefore mixing of substances - entropy growth and anentropy decrease of compounds in the environment.

HA and ***HT*** diagrams can be used in cases where the separation-mixing model is adequate only to a part of occurring changes. This applies to cases of using diagrams in biology, where the number of system elements is the result of many factors, such as reproduction and death.

In nature and in technology, separation of substances occurring at crystal growth of water and silicate solutions (magmas), at differentiation of grains in sizes and density during formation of sedimentary rocks, at composition changes in engineering processes from oil cracking and ore dressing to production of a high-purity chemical reagent, and further up to isotope separation occur with the single ***mechanism of selection***. The very same is used in any reforms in countries; the very same is significant in the evolution of biospecies diversity, in spontaneous and forced changes in national, religious, age, psychological, and other compositions in society.

Dealing with environmental issues is mainly dealing with protection of natural water, atmosphere, soils from their uncontrolled mixing with waste of industry, agriculture, and transport means, respectively, with problems of separation, concentration of these waste components for recycling, utilization or disposal.

In 1918, spelling reform took place in Russia. Writing was "purified" from "excess" elements. To determine the consequences of this action, entropy characteristics of a number of the same texts of various genres, published before and after the reform were measured. It was found that entropy as a measure of diversity – richness of the language decreased [22].

Emergence of a new methodological approach, which includes new terms, types of components, their abbreviations, units of measurement, mathematical formulas, diagrams, methods of material ordering is the stage of mixing – their simultaneous existence with the traditional arsenal of tools for knowledge. System complexity - "The knowledge of multicomponent systems" - has increased.

Work on the method is provided by the software Petros3 developed by S.V. Moshkin. Created mostly for work using RHA method, it includes at the same time a large variety of other data processing methods that enable a comprehensive study of compositional changes. They include several types of diversity measures between compositions. This, in particular, enabled to reveal a significant limitation of the Euclidean distance for work with complex compositions, which include, along with key components, small "admixtures" measured in hundredths and thousandths of a percent. Such compositions are common, for example, in the field of geochemistry, which is often interested in much lower contents. 100 different types of compositions and "composition-like" discrete distributions are possible. [23].

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