ENTROPY METHODOLOGY OF PHYSICO-CHEMICAL PROCESSES

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DOI: https://doi.org/10.56293/IJASR.2022.5531

IJASR 2023
VOLUME 6
ISSUE 3 MAY – JUNE **ISSN: 2581-7876**

Abstract: All phenomena and processes in the nature and world proceed only in two energy directions: either along the force field gradient with minimum energy input (entropy) or against the gradient with maximum energy input (negentropy). The graphs of S-curves and their nomograms characterize the dynamics of change of entropic components depending on the process main parameters. The condition of the system stationary state is the equality or constant of the correlation between its entropy and negentropy (equilibrium dynamics). The entropic methodology functionally provides the basis for physical and chemical regularities in all main scientific fields. The adequate application of geodesic angle in structural interactions can increase the efficiency of the catalysis initial parameters. The concepts presented in the work provide theoretical and practical possibilities to use the entropic methodology in research works and technological innovations.

Keywords: entropy, negentropy, conditions of systems stabilization, S-curves, their diversity, physical and chemical regularities, coronavirus, bioenergetics.

Introduction

In the course of research works in different fields of chemical physics, we can point pout high self-organization and bond between a lot of natural phenomena and processes. For example, Le Chatelier principle in chemical kinetics and N. Bohr complementarity principle in physics, as well as during the analysis of catalysis efficiency parameters. It is obvious that definite general principles and regularities are involved here. Much research has been devoted to the analysis of global processes in living and non-living systems.

An example is the article by G.R. Ivanitsky [1]. In this article, the author believes that the provisions of E. Schrödinger on the ratios of entropy components in a living system are outdated. And for the analysis of global processes in living and non-living matter, he develops the method of chemical kinetics.

This approach, of course, can give effective results, because the nonlinear dynamics of chemical kinetics is in accordance with the principles of directional processes.

For example, this follows from Le Chatelier's principle of chemical kinetics:

"If an external influence is applied to a system that is in equilibrium, the equilibrium will shift in the direction of the process that counteracts this impact."

Thus, the problem of multidimensional manifestation of entropy concept is also of considerable interest. It is known that the concept of entropy, following from the second law of thermodynamics, is the criterion of the process directedness and irregularity degree of systems. Therefore, in this research we try to explain the abovementioned problems from the position of notions of gradient of the directedness of physical and chemical processes during the change in their entropic components.

1. Initial principles

The character of the change in the value of potential energy (ΔU) by its sign was analyzed for different potential fields (Table 1). [2]

Table 1: Directedness of the interaction processes

No	Systems	Type of potential field	Process	U	r_2/r_1 $\left(x_2/x_1\right)$	U_2/U_1	Sign ΔU	Sign δA	Process directedness in potential field
1	opposite electrical charges	electrostatic	attraction	$-k\frac{q_1q_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	-	+	along the gradient
			repulsion	$-k\frac{q_1q_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	+	-	against the gradient
2	similar electrical charges	electrostatic	attraction	$k\frac{q_1q_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	+	-	against the gradient
			repulsion	$k\frac{q_1q_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	-	+	along the gradient
3	elementary masses m_1 and m_2	gravitational	attraction	$-\gamma\frac{m_1m_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	-	+	along the gradient
			repulsion	$-\gamma\frac{m_1m_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	+	-	against the gradient
4	spring deformation	field of elastic forces	compression	$k\frac{\Delta x^2}{2}$	$x_2 < x_1$	$U_2 > U_1$	+	-	against the gradient
			extension	$k\frac{\Delta x^2}{2}$	$x_2 > x_1$	$U_2 > U_1$	+	-	against the gradient
5	photoeffect	electrostatic	repulsion	$k\frac{q_1q_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	-	+	along the gradient

It was found out that the values of $-\Delta U$ and, consequently, $+\delta A$ (positive work) correspond to interactions proceeding along the potential gradient, and $+\Delta U$ and $-\delta A$ (negative work) take place during the interactions against the potential gradient.

After analyzing the first law of thermodynamics, we have the following:

1. In the systems in which the interaction proceeds along the potential gradient (positive work), the resultant potential energy, as well as the reduced mass are found based on the principle of adding reciprocals of corresponding values of subsystems. This is the corpuscular process, in which entropy can serve as the theoretical concept.
2. In the systems in which the interactions proceed against the potential gradient (negative work) the algebraic summation of their masses, as well as the corresponding energies of subsystems is performed. This is the wave process, in which negentropy can serve as the theoretical concept.
3. The resonance stationary state of the systems is fulfilled under the condition of equality of degrees of their corpuscular and wave interactions. In thermodynamics of open systems, the entropy products in stationary state are completely compensated by the negentropy flow.
4. All phenomena and processes in the nature and world, including a human, proceed only in two energy directions: either along the force field gradient with minimum energy input (entropy) or against the gradient with maximum energy input (negentropy). The first direction corresponds to the notion of entropy and the second – to the notion of negentropy (negative entropy). In the dynamics of processes both phenomena are interrelated and complement each other.

2. Entropy nomograms

Heisenberg and Dirac proposed the exchange Hamiltonian derived in the assumption on direct overlapping of wave functions of interacting centers: [3]

$$\overline{H} = -I_0 S_1 S_2 ,$$

where: $\overline{H}$ – spin operator of isotropic exchange interaction for a pair of atoms, I_0 – exchange constant, S_1 and S_2 – overlapping integrals of wave functions.

Each free atomic structure has entropic equilibrium state of two opposite origins (orbital-nucleus) in the system of common reality (atom). Accordingly, in the binary system opposite entropic components from both atoms are interacting until the dynamics of entropic equilibrium stabilizes. Such equilibrium-exchange conformation interactions regulate the stabilization of many organic systems (clusters, polypeptide chains, etc.). Therefore, in this approach the overlapping integrals of wave functions are modeled through the value of relative difference of energy parameters of interacting centers – coefficient α (in %). Such parameter is a direct characteristic of entropic equilibrium degree in the system. The initial values of energy and dimensional parameters for the majority of elements at different valence-active orbitals are given in my other publications. [2,4,5]

Applying the reliable experimental data, we obtain the nomogram of structural interaction degree dependence (ρ) on coefficient α, the same for a wide range of structures (Fig. 1). Here, the values of α from 0 to 5 correspond to the conditions of entropic equilibrium, at which ϱ=100%. This type of nomogram, as well as its dissymmetric variant (Fig. 2) give the possibility to evaluate the degree and direction of the structural interactions of phase formation, isomorphism and solubility processes in multiple systems, including molecular ones. [4,5]

The less is α, the higher is the interaction wave component degree according to Fig. 2 (negentropic curve). And in Fig. 1 the increase of α characterizes the increase in corpuscular and electrostatic properties in microsystems (entropic curve). Thus, the notion of entropy is numerically modeled via coefficient α and negentropy – via 1/ α.

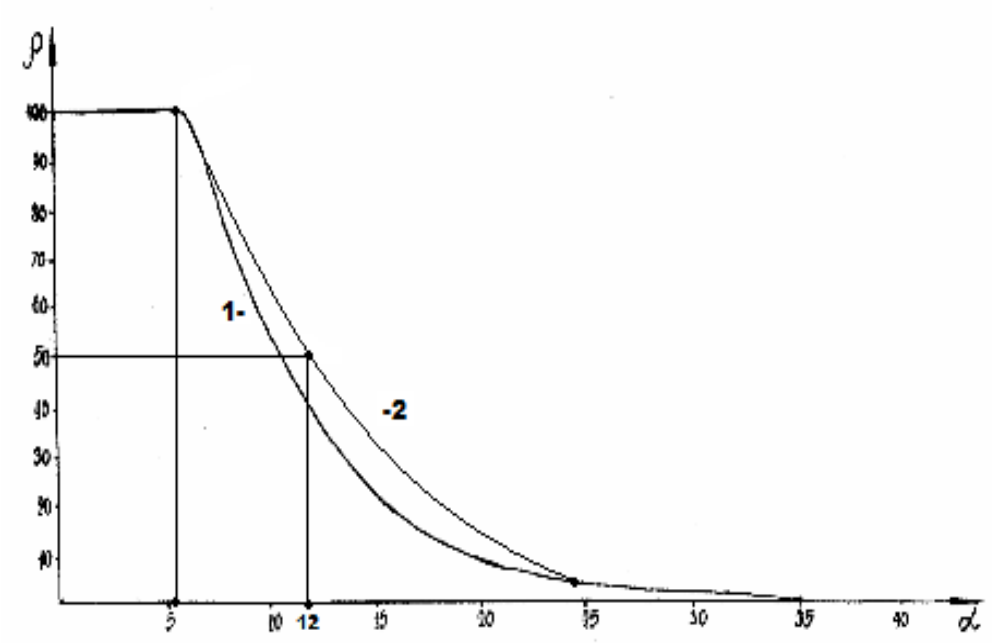

Fig. 1. Nomogram of the dependence of structural interaction degree (ϱ) on coefficient α

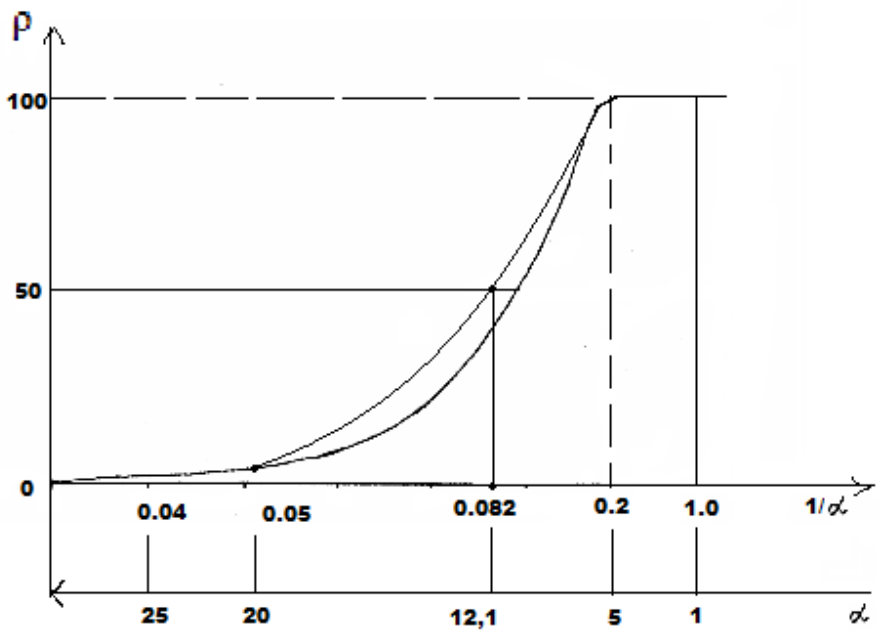

Fig. 2. Nomogram of the dependence of structural interaction degree (ϱ) on coefficient 1/α

Many phenomena and processes in nature, engineering and even economics are described by the same graphs called S-curves. Such S-curves and initial nomograms are graphical characteristics of non-equilibrium dynamics of changes in entropic components.

3. On the conditions of equilibrium and correlations of entropic components.

The execution of point 3 of the initial data is classified depending on the peculiarities of process dynamics. Thus, in electromagnetic wave the difference in the path of vector components is 90°. In general case, during the rotational motion of the system of two similar vectors ($\vec{R}$) with the phase difference of 90° their resultant is as follows:

$$\vec{C} = 2^{1/2}\vec{R}, \text{ where for the given angle } tg45°=1 \quad (1)$$

If such process is complemented by the movement in spiral dynamics, vector ($\vec{C}$) becomes the tangent vector and forms the spiral rotation angle, for which:

$$tg\varphi = C/R = 2^{1/2}, \text{ where geodesic angle } \varphi \text{ equals } 54.733° \quad (2)$$

At this angle a silk worm winds the silk thread onto a base.

Thus, during a purely rotational motion the condition of equilibrium of vector components of entropic characteristics is fulfilled, and during the spiral one their ratio equals $2^{1/2}$. During a translational motion the conditions of either equilibrium or constant ratio of values of their components are fulfilled. At the same time, exponential dependencies are revealed in statistic processes. Such approach defines general principles of many physical regularities.

4. Some examples

1) Characteristic of spin-orbital interaction – fine structure constant $\alpha = \frac{r}{\lambda}$, where r – electron classical radius, λ – its Compton wavelength.

2) In harmonic oscillations of the body the potential energy ratio conditioned by quasi-elastic force to kinetic energy equals $tg^2\delta$, i.e.:

$$E_п/E_к = tg^2\delta \qquad (3),$$

where δ – angular characteristic of oscillations.

If $\delta=\varphi$, the system gets the entropic equilibrium state.

3) Planck's equation (quantum transition):

h = E/ν, where E – orbital energy, constant in stationary state, the process proceeds along the field gradient (entropy), ν – electromagnetic wave frequency (negentropy), h – Planck's constant.

4) Movement velocity equation

V = S/t, where S – way during the mechanical motion with energy consumption (negentropy), t – time, it always increases and is directed along the gradient (entropy). Lorentz curve (the figure is not given) also indicates the availability of space-time dependence. In these cases, the constant motion rate is the condition of stationary state, which is found both in the microcosm of atoms and molecules and in the macrocosm during the movement of planets.

5) From the thermodynamic definition of entropy, it follows that:

T = dw/ds, where dw – thermal energy, therefore, the average temperature (T) is constant both in biological systems and in macrocosm.

6) In this example we use the material from the book. [6]

When manufacturing spaceships, the high-strength thread is wound onto the body at the geodesic angle in compliance with the entropic ratio

$$\frac{\sigma_\beta}{\sigma_\alpha} = \frac{N_\beta}{N_\alpha} = tg^2\varphi = 2 \qquad (4)$$

where: σ_α – axial, σ_β – circumferential stresses are substituted by the proportional value N_α – axial "stress" and N_β – circumferential "stress".

This condition helps obtaining equally strained systems of threads with the minimal item weight.

7) In quantum mechanics the ratio of magnetic moment of the particle to its mechanical moment is called the gyromagnetic ratio g. Here $g_s = 2$, if the electron magnetic moment is conditioned only by the spine component and g = 1, if it is formed by the orbital motion of electrons. Such g values and their ratios characterize the corresponding entropic dependencies.

8) In accordance with the complementarity principle by N. Bohr: for complete description of quantum-mechanical phenomena it is necessary to apply two conflicting (complementary) sets of classical notions, the summation of which provides the exhaustive information about these phenomena as integral ones. For example, the description of an object as a particle and as a wave.

5. On the gravitation mechanism

Newton gravitation model is purely mathematical without any physical content.

Einstein's general theory of relativity (GTR) explains the physical essence of gravitation based on the notion of the change in geometrical properties and distortion of 4-dimensional space – time.

However, according to the modern concept "GTR is not an adequate term and is gradually disappearing from literature being replaced by the "gravitation theory". New theories clarifying the initial principles of GTR emerged. The quantum theory of gravitation is the most fundamental but it is not considered finalized yet. Gravitation is the only fundamental interaction, on which the generally accepted consistent theory has not been constructed yet.

In this work we try to analyze such problems based on the notion of the gradient of directedness of corpuscular-wave processes of different nature.

When a solid (or a mathematical point) rotates around the fixed axis, the vector of total acceleration consists of two vector components: normal acceleration and tangential acceleration.

The vector of normal acceleration at the fixed axis of rotation is directed at it, i.e., along the field gradient. This is a corpuscular part of motion. The vector of tangential acceleration is directed from the system by the tangent to the trajectory, i.e., opposite the field gradient. This is a wave part of the motion.

At the similar motion of charged particles the simultaneous mass and charge transfer takes place. Thus, in the electro diffusion equation of transfer of charged particles the total intensity of flow (J) equals the sum of intensities of mass transfer (J_m) and charge transfer (J_q) :

$$J = J_m + J_q \qquad (5)$$

In compliance with the condition of stationary state (point 3 of the initial data), the action of the corpuscular part defines the wave part of the process. Thus, the rotary motion of charges (corpuscular process) is produced by the magnetic field with its poles (wave process). At the similar motion of the charged particle mass (corpuscular process) the potential field should emerge (wave process). It can be assumed that such field is gravitational with its gravity poles but then there should be a definite ratio between the gravitation and electric constants. Therefore, as applicable to the kinematics of mechanical systems but preserving the formalism of the initial principles, we have: [6]

$$\ln(\frac{G}{\varepsilon_0}) = \mathrm{tg}^2(a_0\varphi) \qquad (6)$$

Where ε_0 – electric constant, G – gravitational constant, $a_0 = 1.00233$ – quantum correction to electron gyromagnetic ratio in an atom, which may, in this case, characterize the influence of particles motion precession. This equation is fulfilled with the deviation from the initial φ value by 0.015%.

Thus, the equation (6) confirms the assumption that the wave contribution of the charged particle mass defines the availability of gravitational field with gravitons as elementary particles.

Therefore, the similarity of Coulomb and Newton equations is not formal, it has physical substantiation. Besides, the similarity of gravitational and inert masses is defined by the equality of the corresponding corpuscular and wave components.

The gravitational force does not depend on chemical composition of bodies or particles. Each body consists of many particles, in the general case, different in nature and size. When the microsystems produce the gravitational field, the process of proton-electron interaction under the action of central forces is common for all structures. In the inanimate nature each system of particles, forming this body, can be considered as a closed one. In such cases (according to point 2 of the initial data) there is a direct algebraic summation of their intensities regardless of the chemical composition of the particles forming the body mass. Besides, the resultant gravitation intensity is directly proportional to the body mass.

But in the animated nature each system is open, therefore, the processes of its interaction with the environment, but with the preservation of specific features of each particle by gravitation, are in progress.

Complex bioenergetic processes go on in any living organism. For example, in DNA molecule during its structural spiral winding and unwinding the direction of such interactions can proceed at the geodesic angle.

The proton-electron interactions between subsystems of this molecule also have the important meaning in DNA conformation dynamics. The gravitational field produced in this process comprises the energy and genetic information from each DNA molecule.

Due to specificity and weak intensity of such field, it is not registered by ordinary instruments but can contact such systems, which can be tuned in resonance with the initial system. This is obviously the main reason of the known effects of a so-called telepathy. But this is a bio gravitational process.

The conclusions on gravitation mechanism

1) The mechanism of gravitation processes was analyzed in corpuscular-wave interactions and in the frameworks of nonrelativistic mechanics using the stationary state condition.
2) The equation of the gravitation constant functional dependence on the electric constant was obtained.
3) It is assumed that gravitation is the wave contribution from the mass of the charged particles during their movement in the field of central forces.

6. S–curves in economics

S-curves are often used in economic investigations, for instance, GDP dynamics, amount and volume of products, forecast of innovation potential, etc. Thus, the graphs [7] of demand line (entropy analogy) and supply line (negentropy analogy) are used to evaluate the rational market price (Fig. 3).

From the graph it is seen that the rational market price is fixed if the demand and supply lines are in equilibrium.

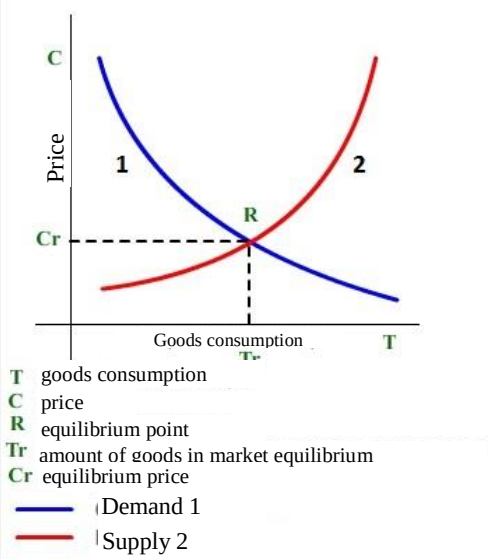

Fig. 3. Graph of demand and supply

7. S-curves in virus etiology

Non-equilibrium dynamics can be also demonstrated in virus etiology, which can be interpreted as smooth transition from atomic-molecular interactions on the microlevel to a formally similar process in macrosystems. This analogy is confirmed by the graph (Fig. 4) for the Russian coronavirus scenario in its most aggressive period before the omicron virus emergence. [8]

Using the comparative methods with reference nomograms, we can make some assumptions about further progress of the coronavirus scenario. [9]

Fig. 4. Number of diseases in the given time period.

8. Bioenergetics of living systems

Entropic principles of bioenergetics of live systems define a wide range of their functional capabilities. And first of all – life span. Longevity problems have always been studied and investigated in the world and their results have been considered and applied at different times, though with various degrees of success. Gene-protectors, normalizing the dysfunction of organs, are currently applied to prolong a human's life. [10] Such problematic issues can be considered from the position of principles of entropic correlations.

The equality or parity correlation of these entropic parameters is the condition of any static stability of any system. The heart works this way: work phase (systole) is always accompanied by functionally equal rest phase (diastole). Therefore, the following principle is fulfilled for the stable live system: physical activity and movement should be adequately compensated by leisure and rest. And vice versa. Similarly in nutrition energetics: the amount of calories absorbed should equal the amount of calories spent.

Conclusion

This approach of applying the entropic methodology is not brand new and the given examples are not single. In 1943 E. Schrodinger in his book "What is life?" explained that in a live system the negative entropy produced by a body balances the positive entropy flow. Thus, thousands of years ago Chinese medicine considered all phenomena of the world and nature as the interaction of two opposite geneses of unified reality. And the principle of unity and struggle of opposites is fulfilled in dialectics.

From the point of these ideas, physiotherapy and reflex therapy can be considered as the methodology of equalizing the potentials of two manifestations of energy geneses, which are the entropy and negentropy. And the nature today, as before, fulfills its principles. For example, it struggles against viruses by collective immunity.

At present, in the time of ecological problems, there is an important principle: all carbon dioxide produced must be absorbed.

Since the initial principles of these regularities are unknown for broad scientific community, their application in practice is evidently insufficient. But it is necessary to take these principles into account in the technology of producing hybrid products consisting of two or more components (or fractions). The products obtained this way will have better quality than the ordinary ones.

This methodology has a special meaning in material science. In such cases, the problematic issues of phase-formation and extension of solid solutions arise. This approach allows finding the optimum solutions to evaluate the interaction degree of atomic-molecular structures.

General conclusions:

1) the entropic methodology functionally provides the basis for physical and chemical regularities in all main scientific fields.
2) the adequate application of geodesic angle in structural interactions can increase the efficiency of the initial energy parameters.
3) the concepts presented in the work provide theoretical and practical possibilities to use the entropic methodology in research works and technological innovations.

References

1. Ivanitsky G. R. "21st century: what is life from the point of view of a physicist?" Uspekhi fizicheskikh nauk, volume 180, number 4, 2010, p. 337-369
2. Korablev G.A. Spatial-energy interactions. Monograph, Stary Oskol: TNT, 2018, 132 p.
3. P.A. Dirac, Quantum Mechanics, London, Oxford Univ., Press, 1935.
4. Korablev G.A. Diversified Demonstration of Entropy / Korablev G.A., Petrova N.G., Osipov A.K. et al. // New Book Announcement. Nanotechnologies to Nano industry. - USA, Winter 2013/14. - Chapter 8. P. 120-130.
5. Korablev G.A., Zaikov G.E. Bio-structural energy criteria of functional states. News of HEIs. Applied chemistry and bio-engineering. 2012, v. 1(2), p. 118-124.
6. Kodolov V.I. Polymeric compositions and technology of producing aircraft engines from them. Izhevsk Mechanical Institute, 1992. – 200 p.
7. Business ideas for home production [Electronic source] URL: https://businessideas.com.ua (reference date: 02.10.2020).
8. Wikipedia. COVID-19 pandemic in Russia [Electronic source] URL: https://wikipedia.org/wiki/COVID-19_pandemic_in_Russia (reference date: 02.10.2020).
9. Korablev G.A. Virus entropic characteristics / Korablev G.A. // EIJASR Journal 2020 vol-3, issue - 3, may-june, p / 146-152.
10. M.S. Pristrom, B.E. Sushinsky, I.I. Semenkov, E.P. Vorobieva. Physiological and premature ageing. Place of statins in preventing premature ageing // Medical news: journal. – 2009, iss. 6, p. 25-30.