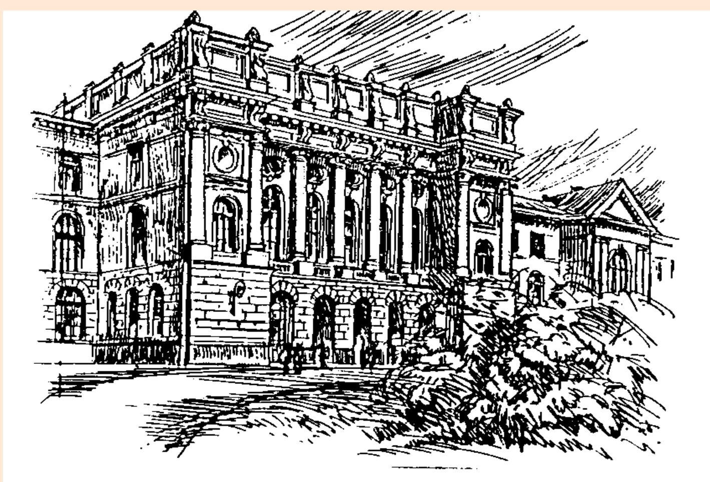

Information - Statistical Approach to Inverse Optical Problem Solution for *3D* Disperse Systems with Nano and Micro Particles

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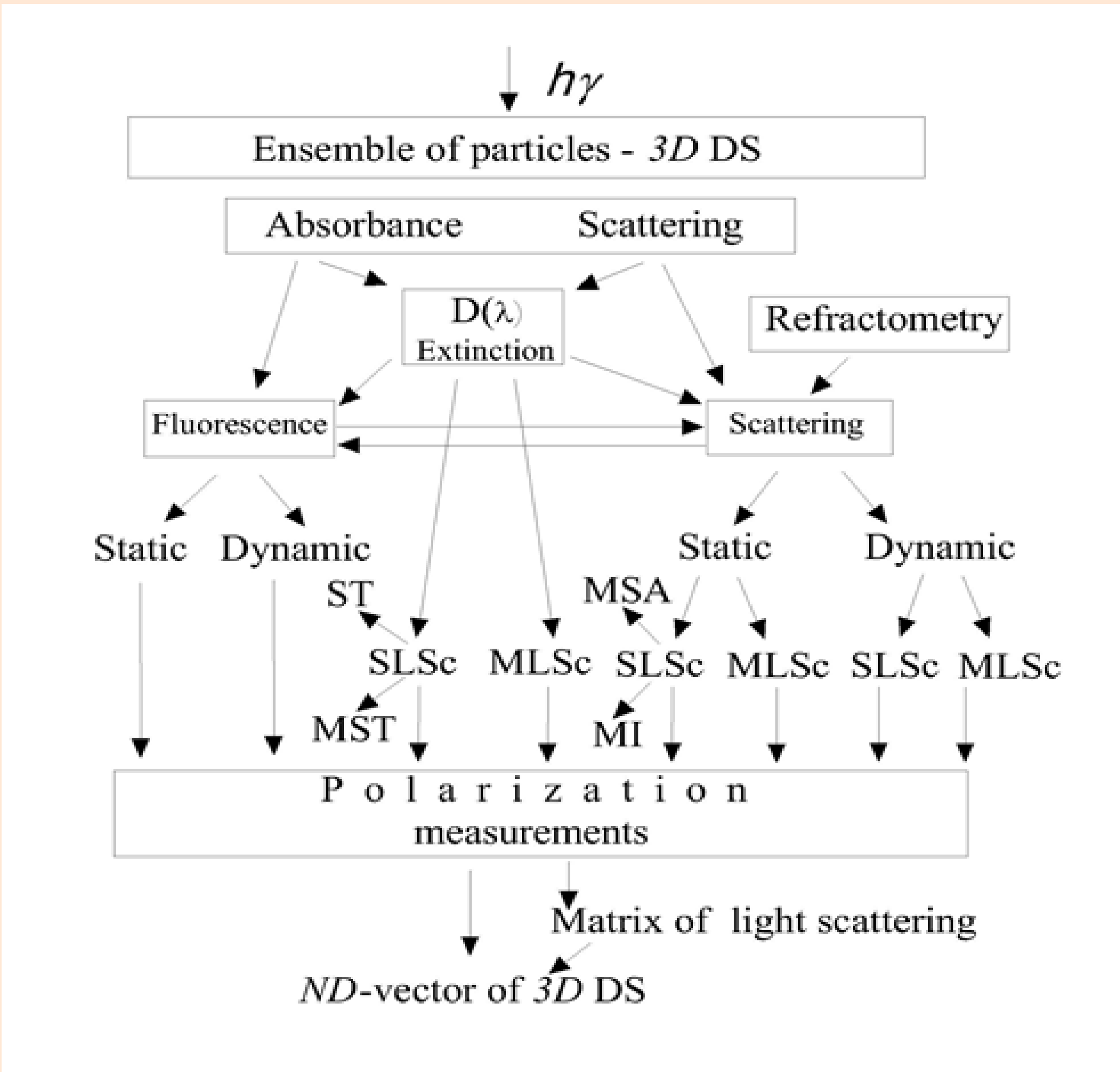
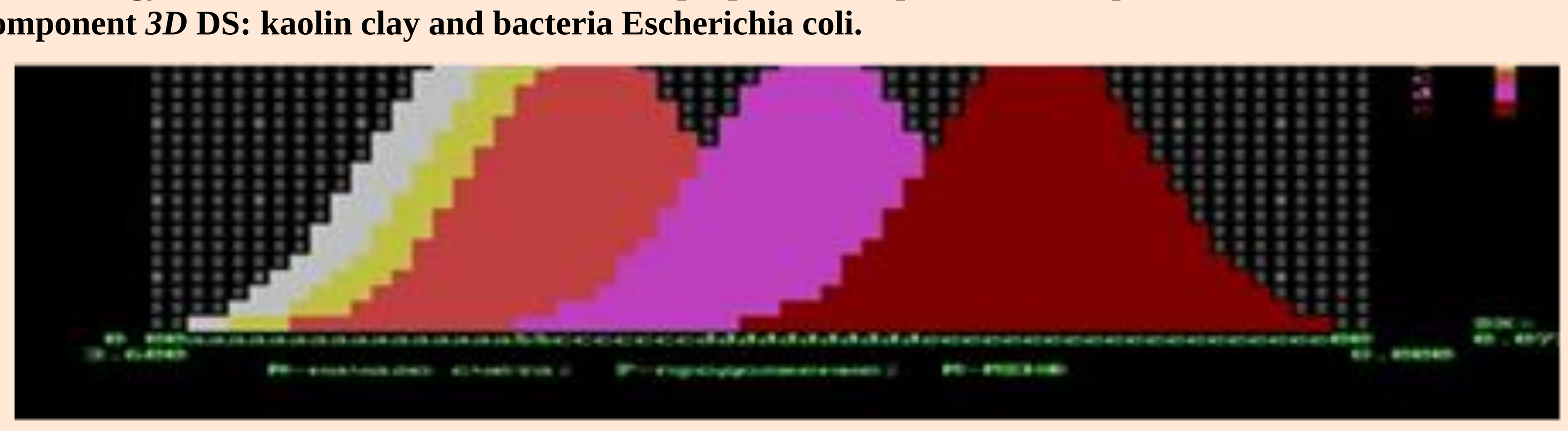


Fig. 1. Scheme of compatible optical methods for *3D* DS characterization [6]. Abbreviations: SLSc - singular light scattering, MLSc - multiple light scattering. Methods of solving the inverse optical problems: ST- spectroturbidimetry [1] , MST- method of spectral transparency, MSA- method of small angles, MI- method of indicatrix.

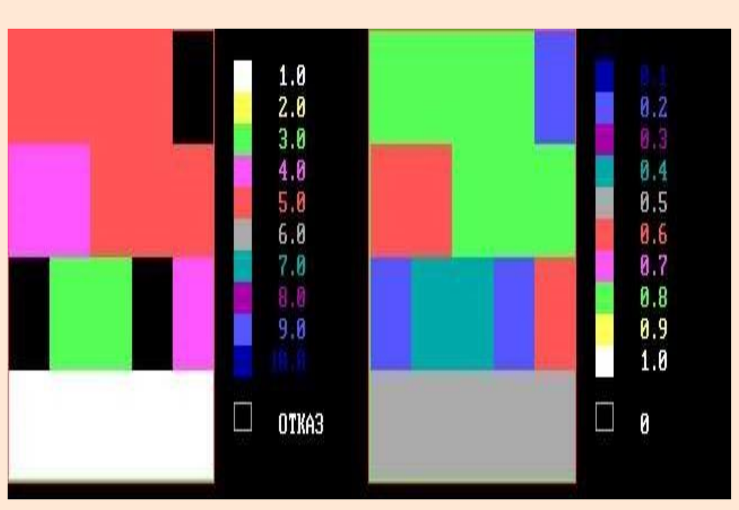
***ND*-vector of *3D* DS [2 – 7] is the set of the "second-class" optical parameters, which can be online calculated from experimental optical data without "a priori" information about particles (for example, wave exponent - n [1] or light scattering matrix elements [5]) and are mainly independent from particle concentration.**

The following water *3D* DS (dispersions, colloids, suspensions, with diameter less than 10 micro-meters) were studied: proteins, nucleoproteins, lipoproteids, liposomes, viruses, fat emulsions, perfluorine carbons-based blood substitutes, antibiotics, nanoparticles of polycyclic aromatic hydrocarbons, cyclodextrins, latexes, liquid crystals, bacterial and another biological cells with various form, size, strains (coli bacillus, lactobacillus, thrombocytes, erythrocytes and erythrocyte diagnosticums, lymphocytes and thymocytes, Ehrlich ascites carcinoma cells, etc.), metal powders, kaolin, kimberlites, zeolites, etc., and mixtures - proteins and nucleic acids, proteins and polymers, liposomes and viruses, liposomes carrying various substances (X-ray contrast agents, metallic particles, enzymes, viruses, antibiotics, etc.), liquid crystals with surfactants, mixtures of coli bacillus with kaolin, mixtures of anthracene with cyclodextrin, oils, milk, samples of food, samples of natural and water-supply waters, air sediments in water, etc. For the solution of inverse optical problem, the different approximations of particle form were used such as spheres, prolate and oblate ellipsoids of rotation, core / shell spheres.

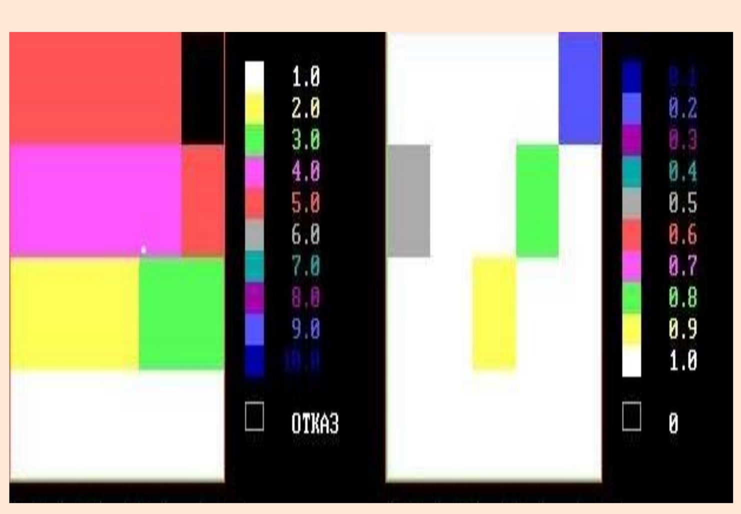
For biomedical and natural *3D* DS of micro- and nano- particles (water, blood, vaccines, etc.) the solution of inverse optical problems meets with difficulties connected with polymodality of particle size distribution and polycomponent content of systems. Information-statistical theory algorithms allow by comparison of unknown *3D* DS *ND*-vector with known one from Data bank to estimate the probability of presence in system the component of interest. For this goal a software package MULTALT [10] was used providing the process of interpretation and visualization of intermediate and final results with estimation of decision probability. The methodology was tested on mixed in different proportions experimental dispersions consisted of two mono-component *3D* DS: kaolin clay and bacteria Escherichia coli.



a)



b)



c)

Fig. 2. Example of five-alternative problem for five *3D* DS: a) example of "second class" parameter distributions - clay (a-1-white), Escherichia coli bacillus (a-5 -burgundy color) and their mixtures as the concentration of cells increases (2, 3, 4); b) and c): solutions (left) with solution probabilities (right) for all dispersions based on experimental parameters of second class: b) one parameter and c) complex of five parameters. The number of parameters in complex can be enlarge and it will be possible to find the optimal complex of parameters for determination of interest components. "OTKA3" means program refuse from solution with probability 0,2

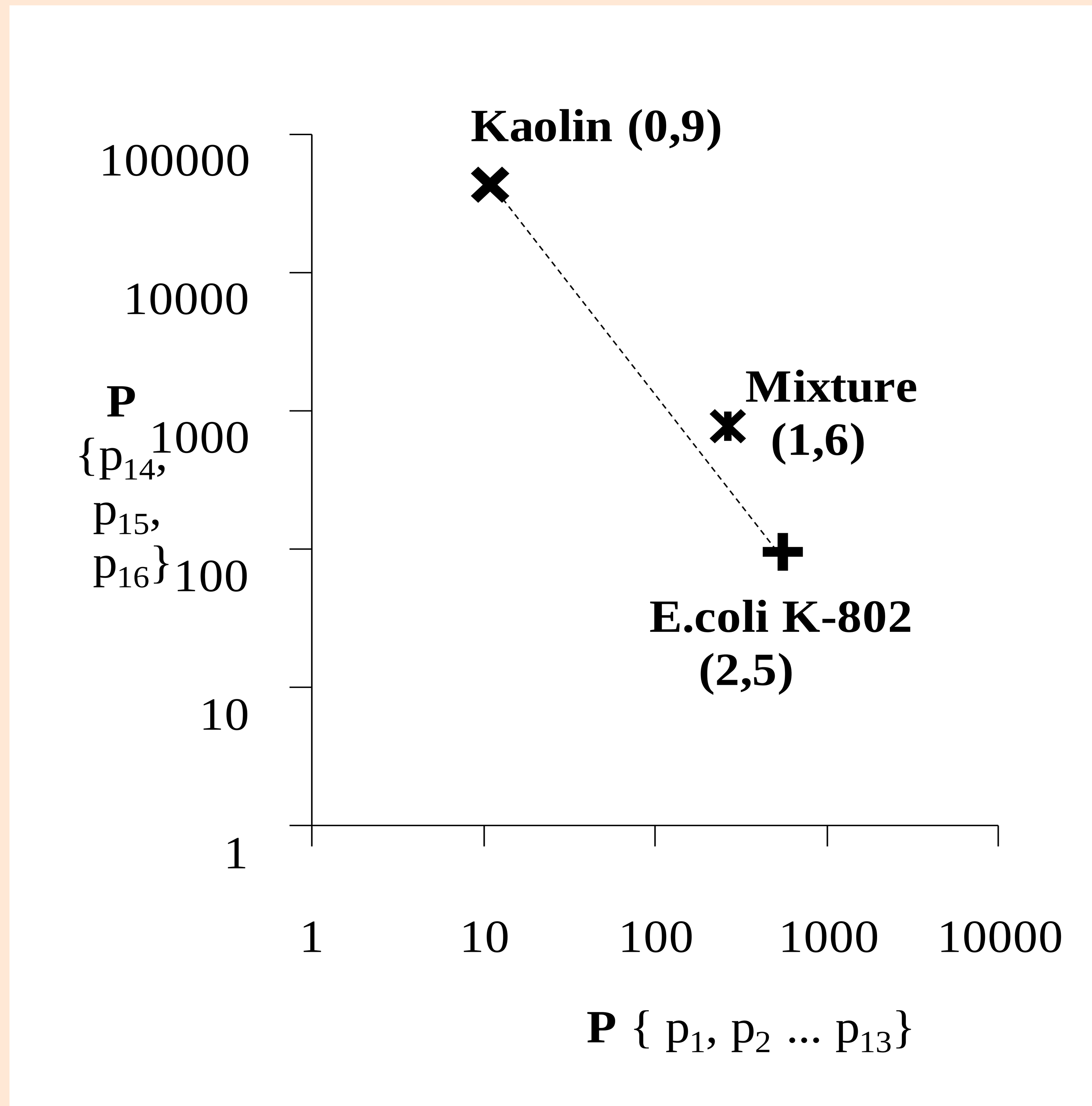


Fig. 3 . The optical characteristics as *16D*-vectors P {p_1, p_2, … p_{13}, p_{14}, p_{15}, p_{16}} for: dispersion of E.coli (+) strain K-802 with n (500) = 2,5, kaolin dispersion (x) with n (500) = 0,9 and their mixture (ж) in ratio 1:1 by volume with n (500) = 1,6. All p_i are parameters of second class and do not depend from concentration of particles. Measurements of dispersions were made at the same conditions. The uncertainty is about 7%. Numbers in brackets are the values of n at 500 nm for corresponding dispersions [5].

Multiparameter optical characterization of *3D* DS includes: a) the simultaneous measurements of dispersion by different compatible non-destructive optical methods such as refractometry, absorbance, fluorescence, light scattering (integral and differential, static and dynamic, unpolarized and polarized), b) solution of inverse optical problem by different methods among which are technologies for the data interpretation by the information-statistical theory. Characterization of *3D* DS by different compatible nondestructive optical methods is desirable because of possibility to organize the *on-line* control. At the information–statistical approach to the *3D* DS optical control, it is possible to qualify the *3D* DS state changes under different conditions by *N*-dimensional vectors of optical parameters of second class (*ND*-vectors). The experience suggests [2-8] that the *set* of "second class" optical parameters (*ND*-vector) can be unique for each *3D* DS and can reflect in "unobvious" form all peculiarities of *3D* DS: nature (constituent substances), form, inner and surface structure of particles, distributions of particle size, number, mass, refractive index, form, structure, tendencies (liability) to aggregation, coalescence, changes in the state of mixtures, etc. Due to the fusion of various optical data and by information statistical methodology, it is possible to find the set of the most informative parameters for *3D* DS state *on-line* differentiation and to solve the inverse optical problem on the presence of a component of interest in mixtures. This approach can be considered as an integral one for the control of system at the moment of measurements as *a single whole intact unity*. It can demonstrate an awareness of potential applications for bio- and nanotechnology, drug delivery, colloid science, etc. and for protection of environment.

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