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OPTICAL CHARACTERIZATION OF *3D* DISPERSE SYSTEMS WITH NANO- AND MICRO PARTICLES: LIGHT SCATTERING MATRIX ELEMENTS

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Abstract. The multiparametric analysis of simultaneous optical data for nano and micro particle systems (ensembles, colloids, dispersions) by presentation of system characteristics as *N*-dimensional optical parameter vectors can help to elucidate differences or changes in the state of particles, the process of particle interactions, the particle share in mixtures and so on. In this paper, the light scattering matrix elements application as vector parameters is shown on the examples of influenza virus and colibacillus dispersions. These optical parameter *ND* vectors can serve as the innovative research platform for sensing different particle interfaces including biological ones.

1. Introduction

Ensembles of nano- and / or micro particles can be considered as three-dimensional (*3D*) disperse systems (DS) with particles as a disperse phase in dispersive medium [1]. Multiparametric analysis of optical data for *3D* DS can provide further progress for detailed characterization and control of *3D* DS with particles of different nature (including biological ones). Taking into account optical theory [1-4] and results of experiments [5-20] can help to elaborate sensing elements for on-line control of *3D* DS state. In our research [5-19] we have investigated different *3D* DS with nano- and / or micro particles (with diameter less than 10 micrometers). It has included: a) simultaneous measurements of *3D* DS by different compatible nondestructive optical methods such as refractometry, absorbance, fluorescence, light scattering (integral and differential, static and dynamic, unpolarized and polarized), and b) solution of inverse optical problem by different methods, and technologies of data interpretation by information-statistical theory [21]. The experience suggests that the set of optical parameters of so-called “second class” is unique for each *3D* DS. In other words, each *3D* DS can be characterized by *N*-dimensional vector in the *N*-dimensional space of the “second class” optical parameters (*ND* vector) [13]. *ND* vectors 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, etc.; possibilities to aggregation, destruction or interaction with another particles, and so on.

The light scattering matrix elements [2-4, 20] being “second class” parameters by definition (obtained by processing of measured values, dimensionless, mainly independent on the concentration of particles) are very perspective for multiparametric analysis of *3D* DS. In this paper the application of light scattering matrix elements as *ND* vector parameters (alone

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and in complex with "second class" parameters from other optical methods) is shown on the example of such biological *3D* DS as colibacillus and influenza virus dispersions.

2. Materials and methods

The form of influenza virus particle can be approximated as a homogeneous sphere, but in some cases, the bilayered sphere approximation can be useful. Colibacillus bacterial cell (Escherichia coli, E. coli, colibacillus rods) can be approximated as a homogeneous volume-equivalent sphere and as a prolate ellipsoid of rotation [4]. In this paper the influenza virus strain A1 - H1N1 with mean diameter of particles 100 nm and dispersions of colibacillus with equivalent-volume sphere mean diameter of cells 1.0 μm (strain K-802) and 1.3 μm (strain AB 1157) were used. Due to the great sensitivity of biological objects to the surrounding medium and conditions, it is necessary to use simultaneous measurements for comparison of objects and to take into account all details of experiments (pH, content of nutrition medium, temperature, etc.).

In the previous articles [19, 20] there is the description of main optical methods used for *3D* DS characterization: *refractometry, fluorescence, absorbency, integral light scattering, differential static* and *dynamic light scattering.* For the measurements of light scattering matrix elements, laser (wavelength 633 nm) self-made installation with detector angles from 60 up to 120 degrees, polarizer and retardation element [2] was used.

3. Results and discussion

The Stokes vector **F** describes the complete polarization properties of a beam of light. The effect of scattering on a beam of light can be represented by the Mueller matrix M (with 16 dimensionless elements S_{ij}), that transforms the Stokes vector for the incident light $\mathbf{F}_{inc}$ into the Stokes vector representing the scattered light $\mathbf{F}_{sc}$ [2, 3]:

$$\mathbf{F}_{sc} = \mathrm{M}\,\mathbf{F}.$$

Here $\mathbf{F}_{inc}$ is the Stokes vector for the incident light, $\mathbf{F}_{sc}$ is the Stokes vector for the scattered light, M is 16-element Mueller matrix:

$$\mathrm{M} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{bmatrix},$$

S_{ij} are the functions of the scattering angle which contain all information about the elastic light scattering properties of a particle system at a given wavelength [2-4, 20]. In Fig. 1 an example of light scattering S_{34} matrix elements angular dependence is given (modified experimental data from classical work [20]) for dispersions of two colibacillus strains is presented. The scattering matrix is determined by the size, shape, symmetry, internal structure and optical properties of the particles in system. In general, all 16 dimensionless elements of the scattering matrix for nonspherical particles can be nonzero and depend on orientation of the scattering plane. The *3D* DS state characterization as *ND* vector can be implemented in the *N*-dimensional space of matrix elements alone (Fig. 2) or in the complex with other optical parameters (Fig. 3 and Fig. 4). The first case can be demonstrated on the example of S_{34} matrix elements experimental data for two strains of coli bacillus published in classical work [20]. The published data on angular dependences of S_{34} / S_{11} for E. coli strain B/r [20, Fig. 5a] and strain K-12 [20, Fig. 5b] were processing according *ND* vector approach: the most informative eight parameters were found for differentiation of dispersions state by several orders (Fig. 2, a-c) and by sign (Fig. 2, d).

In our research (Fig. 3), the *3D* DS state characterization as *ND* vector in the *N*-dimensional space of matrix elements in complex with other optical parameters was used in order to design optimal scheme for dispersions on-line control: the S_{11} angular data for E. coli strain K-802 and strain AB1157 was combined with integral light scattering data (Fig. 3). For data in Fig. 3, measurements of dispersions (4 dispersions for each strain) were made at the same conditions. The uncertainty is about 10%. It can be concluded from Fig. 3 that P_l and P_m are less informative parameters than P_i and P_k, and it is necessary to find more informative "second class" parameters for differentiation of these *3D* DS.

The bilogarithmical plots in Fig. 4 are the examples of optical data presentation in the *12D* (Fig. 4a), *4D* (Fig. 4b) and *16D* (Fig. 4c) spaces of optical parameters for dispersions of influenza virus (strain A1-H1N1) and colibacillus cells (strain K-802). Taking into account the angular dependences of S_{11} (parameters denoted with subscription S) and S_{12} (parameters denoted with subscription P) it is possible to form *ND* optical parameter vectors $\mathbf{P_S}$ $\{P_{S1}, P_{S2}, \ldots P_{SN}\}$ and $\mathbf{P_P}$ $\{P_{P1}, P_{P2}, \ldots P_{PN}\}$ correspondingly (Fig. 4a, where N=6). In Fig. 4b, the four informative "second class" optical parameters from integral and differential static light scattering, P_1, P_2, P_3. P_4, are presented. The complex *16D* vectors (from Fig. 4a and Fig. 4b) are given in Fig. 4c. It can be seen that the difference in positions of E. coli and influenza virus dispersion characteristics is significant.

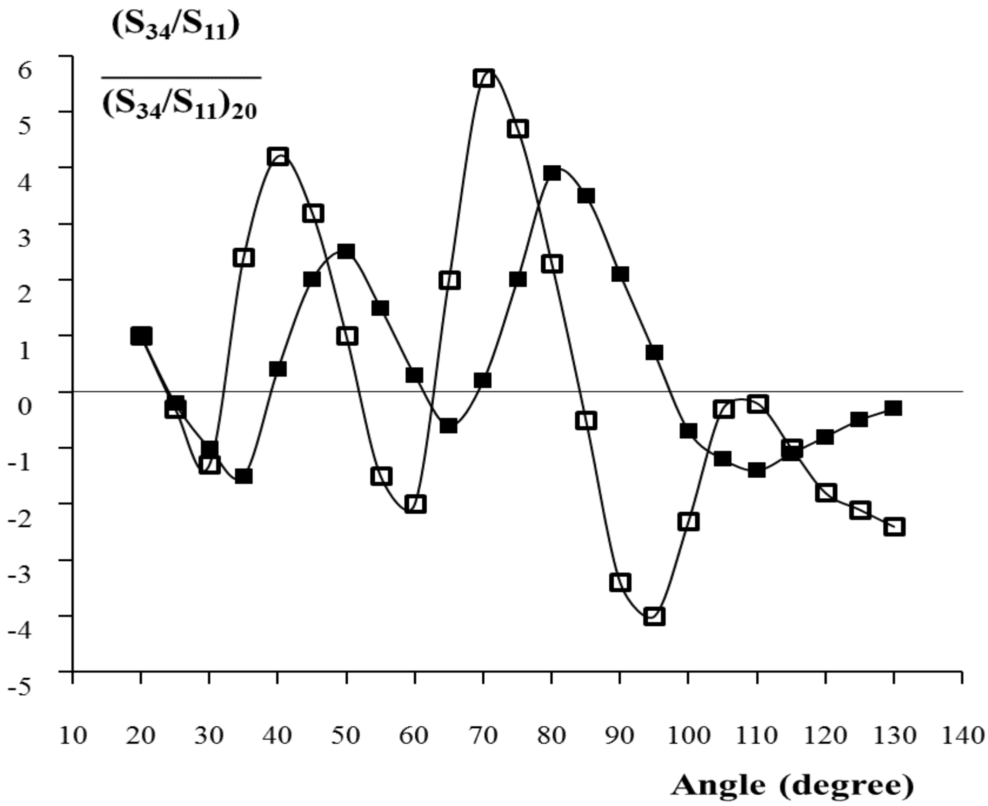

Fig. 1. Example of light scattering S_{34} matrix elements angular dependence (modified and normalized at angle 20^0 data from classical work [20]) for dispersions of two colibacillus strains: ■ - strain B/r, □ - strain K-12.

The classical experimental data [20] about angular dependences of S_{34} / S_{11} for E. coli strains B/r and K-12 were processing according *N*-vector approach for differentiation of dispersion states by several orders (Fig. 2a-c) and by sign (Fig. 2d).

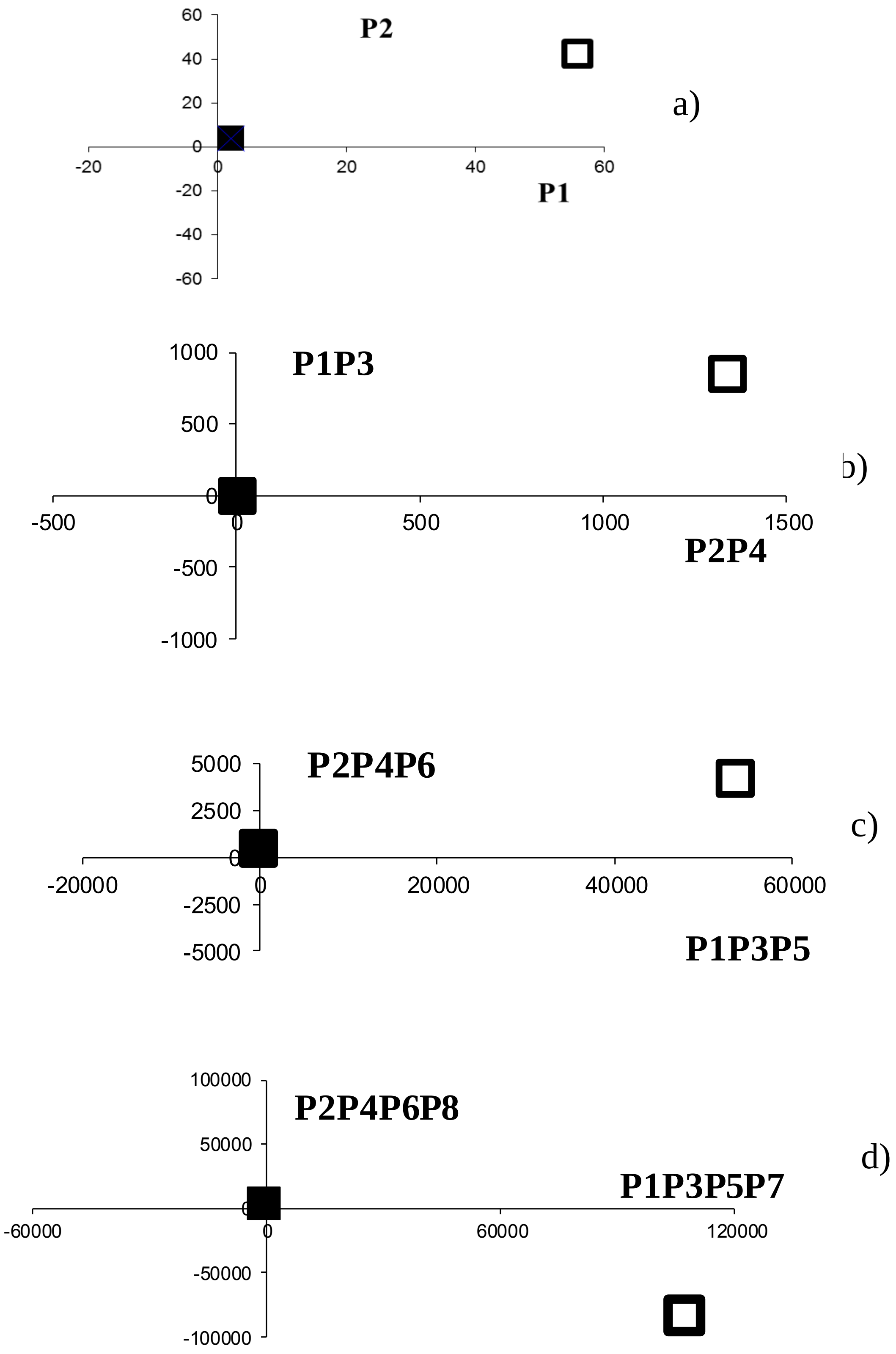

Fig. 2. Optical parameter *N*D vector presentations in the *N*D spaces of S_{34} light scattering matrix elements for dispersions of two colibacillus strains as the result of Fig. 1 data processing: a) N=2, b) N=4, c) N=6, d) N=8; ■ - strain B/r, □ - strain K-12.

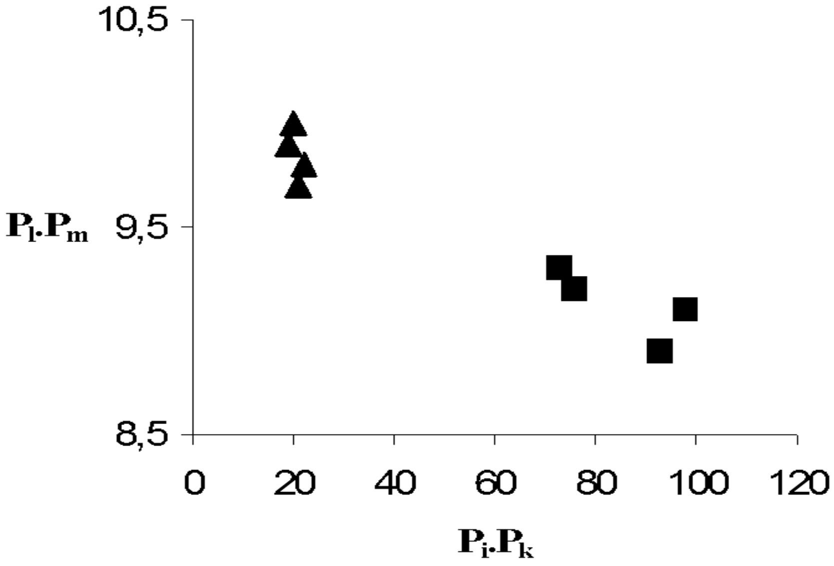

Fig. 3. Example of optical parameter *ND* vector presentation for dispersions of Escherichia coli two strains (K-802 - ▲, AB 1157 - ■) as *4D* vectors **P** {P_i , P_k , P_l , P_m} in *4D* space of “second class” optical parameters (including S_{11}) without any *a priori* information about cell structures and size distributions. Optical parameters are independent of cell concentration.

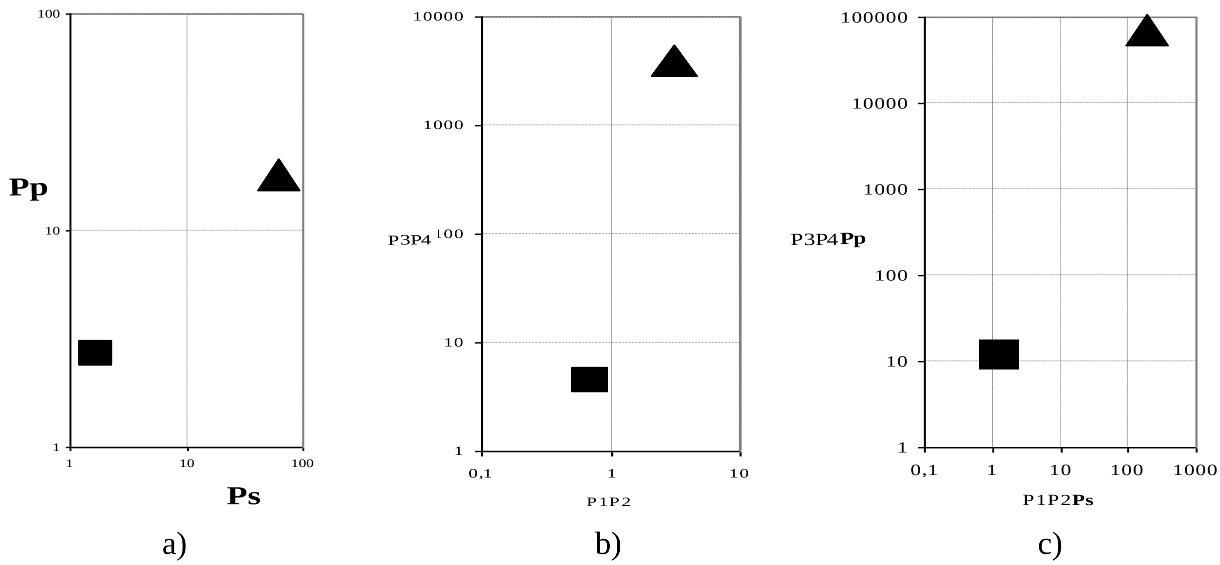

Fig. 4. Bilogarithmical plots as examples of optical parameter *ND* vector presentations for dispersions of influenza virus (strain A1-H1N1 - ▲) and colibacillus cells (strain K-802 - ■): a) as *12D* vectors $\mathbf{P_{SP}}$ {P_{S1} , P_{S2} ,… P_{S6} , P_{P1} , P_{P2} ,… P_{P6}}, parameters denoted with subscriptions S and P were obtained from angular dependences of light scattering matrix elements S_{11} and S_{12} correspondingly; b) as *4D* vectors $\mathbf{P_4}$ {P_1 , P_2 , P_3 , P_4}, parameters from integral and differential static light scattering; c) as *16D* vectors $\mathbf{P_{16}}$ {P_1 , P_2 , P_{S1} , P_{S2} ,… P_{S6}, P_3 , P_4 , P_{P1} , P_{P2} ,… P_{P6}}. Optical data are independent of concentration of virus and cell particles.

4. Conclusion

Optical parameter *ND* vectors can reflect in "unobvious" form many peculiarities of a system state. The *3D* DS can be characterized and compared with each other by means of the *ND* vectors. The vectors can also reflect the changes in the state of mixtures. Due to the fusion of various optical data and by the information statistical theory, it is possible to find the set of the most informative parameters and to solve the inverse physical problem on the presence of the component of interest in mixtures without any regularization. In this case, the polymodality of particle size distributions [19] is not an obstacle.

The number of parameters can be enlarged if to consider angular (Fig. 2, Fig. 4a) and wavelength dependences of experimental optical data. Optical parameter *ND* vector approach can be considered as "integral" for the study of a whole system as unity with the minimum interference. The presentation of *3D* DS characteristics as optical parameter *ND* vectors can serve as the innovative research platform for sensing of particle interfaces. It also can demonstrate an awareness of the potential applications for bio- and nano-technology, medicine, industry and for the protection of environment.

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