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
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 \( \mathbf{F} \) 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 \( \mathbf{M} \) (with
16 dimensionless elements \( S_{ij} \)), that transforms the Stokes vector for the incident light \( \mathbf{F}_{\text{inc}} \) into
the Stokes vector representing the scattered light \( \mathbf{F}_{\text{sc}} \) [2, 3]:

\[
\mathbf{F}_{\text{sc}} = \mathbf{M} \mathbf{F}_{\text{inc}}
\]

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

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

\( S_{ij} \) 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 $P_S \{P_{S1}, P_{S2}, \ldots, P_{SN}\}$ and $P_P \{P_{P1}, P_{P2}, \ldots, P_{PN}\}$ 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](image_url)

**Fig. 1.** Example of light scattering $S_{34}$ matrix elements angular dependence (modified and normalized at angle $20^\circ$ 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 ND vector presentations in the ND 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 $P_1$, $P_k$, $P_i$, $P_m$ 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 $P_{SP}$ [$P_{S1}$, $P_{S2}$, ..., $P_{S6}$, $P_{P1}$, $P_{P2}$, ..., $P_{P6}$], 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 $P_4$ [$P_1$, $P_2$, $P_3$, $P_4$], parameters from integral and differential static light scattering; c) as 16D vectors $P_{16}$ [$P_1$, $P_2$, $P_{S1}$, $P_{S2}$, ..., $P_{S6}$, $P_3$, $P_4$, $P_{P1}$, $P_{P2}$, ..., $P_{P6}$]. 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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