UDK 543.087.9

SHANNON ENTROPY AS A CHARACTERISTS OF COMPLEX REACTION-DIFFUSION SYSTEMS

Timralieva A.A. (ITMO University), Aliev T.A. (ITMO University), Nesterov P.V. (ITMO University)

Scientific supervisor – Prof. Dr. Skorb E.V

(ITMO University)

Convolutional neural networks opened the way to determine the changes of complex chemical systems by the analysis of different source images such as high-speed camera images [1] and optical microscopy images [2]. These neural networks can classify images into specified classes using the image pattern recognition [3]. However, there is still a problem to describe the complex system. The only way is to use mathematical statistics and further visualization of the data. This approach is not suitable enough as it is rarely clearly representative.

We propose to use new parameter that is based on the statistics such as Shannon entropy. This parameter initially indicates the unpredictability of symbol's appearance in an alphabet. We propose to use Shannon entropy to define the appearance of spherical capsules with certain diameter. Herein we characterize reaction-diffusion systems with melamine cyanurate capsules formed in presence of different dyes as the size of capsules differs in these cases. We also varied the concentration of melamine and cyanuric acid in the system also as the distance between initial compounds.

Thus, we obtained Shannon entropy values for several reaction-diffusion systems and estimated the efficiency and representativity of this parameter as an additional estimation value for complex systems.

References:

1. Korolev I. et al. When Bubbles Are Not Spherical: Artificial Intelligence Analysis of Ultrasonic Cavitation Bubbles in Solutions of Varying Concentrations // J Phys Chem B. American Chemical Society, 2022. Vol. 126, № 16. P. 3161–3169.
2. Aliev T.A. et al. Designed assembly and disassembly of DNA in supramolecular structure: From ion regulated nuclear formation and machine learning recognition to running DNA cascade // Nano Select. John Wiley & Sons, Ltd, 2022. Vol. 3, № 11. P. 1526–1536.
3. Sharma N., Jain V., Mishra A. An Analysis Of Convolutional Neural Networks For Image Classification // Procedia Comput Sci. 2018. Vol. 132. P. 377–384.