Digital modeling of of biodegradable polymers characteristics using the example of compositions based on low density polyethylene with natural rubber

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Abstract.

One of the most important tasks in the implementation of the concept of sustainable development and formation of "Green Economy" is the wider use of biodegradable materials that reduce the negative impact on the environment. It is especially true in the view of accumulation of synthetic polymer waste in the environment, primarily polyolefins, which have exceptional resistance to physicochemical and biological degradation. Currently, one of the most promising directions in the development of biodegradable materials is the creation of compositions based on low density polyethylene with various products of plant origin, such as sawdust, flaxseed fire, natural rubber. At the same time, depending on the content of natural additives in such materials, a line of biodegradable materials can be obtained from several compositions that differ in physical and mechanical properties and in the degree of biodegradation. As it was revealed by the authors in the framework of previous studies for various compositions based on low density polyethylene with natural rubber and their comparative analysis with other compositions based on low density polyethylene with various products of plant origin, the change in properties in the process of degradation of such biopolymers has a complex nonlinear character and changes over a long period of time (up to 18 months). Thus, the issue of modeling the degradation properties of biopolymers and the creation of a library of digital twins of various compositions based on low density polyethylene with various products of plant origin, taking into account the requirements for the physicochemical properties of the obtained polymers, becomes highly relevant.

To solve this problem, the authors approximated the experimental biodegradation curves using the example of compositions based on low density polyethylene with natural rubber and identified regressors for constructing approximating functions for various compositions. The resulting models showed high accuracy in relation to experimental values (the value of the coefficient of determination was about 0.85). The use of the developed mathematical models will significantly reduce the time spent on the development of new biopolymer compositions with the required level of biodegradation and the required physicochemical properties. In addition, taking into account the high share of material costs in the production cost of composites based on low density polyethylene with various products of plant origin, the use of mathematical modeling will make it possible to estimate their cost for potential consumers.