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ВЫБОРОЧНЫЕ СРЕДСТВА СИСТЕМНОГО АНАЛИЗА ДЛЯ ИДЕНТИФИКАЦИИ СВОЙСТВ АКТИВНЫХ ИНГРЕДИЕНТОВ В СОСТАВЕ ПОЛИМЕРНЫХ КОМПОЗИЦИЙ

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Проведен обзор работ, использующих квантово-химические и другие методы математического моделирования для идентификации и управления свойствами полимерных композиций. Рассмотрены некоторые неэмпирические методы, а также методы DFT и их роль в современных исследованиях. Выделены основные этапы оценки свойств полимерных композиций. Среди них анализ «структура-свойства», управление свойствами полимерных композиций как во время полимеризации, так и с помощью варьирования активных и пассивных добавок. Рассмотрены основные тенденции использования математического моделирования для решения подобных задач. Проведен анализ современных подходов, применяемых для исследования свойств, среди которых можно выделить нейронные сети и методы, требующие высокопроизводительных вычислений. Подробно описаны некоторые из моделей, например, фундаментальные уравнения терминальной модели и модели предпоследней единицы. Среди примеров также указаны: метод клеточных автоматов, математическая модель воздействия переменного электрического поля на композит, метод моментов для расчета средней молекулярной массы полимера, уравнения, описывающие процесс полимеризации для высокомолекулярных соединений. В данном обзоре также было проанализировано новое перспективное направление использования нанокомпозитов, участвующих в синтезе новых долговечных продуктов, обладающих улучшенными свойствами. Проведенная работа показала, что даже на одних и тех же этапах оценки свойств полимерных композиций используются совершенно разные как квантовохимические, так и другие математические методы. Рассмотренные в данной работе математические методы можно систематизировать в три группы: моделирование зависимости «структура - свойство», управление свойствами при синтезе полимеров, управление свойствами композиционных материалов путем изменения компонентов этой композиции.

Ключевые слова: квантовая химия, математическое моделирование, композиционные материалы, полимерные композиции, нанокомпозиты

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SELECTIVE SYSTEM ANALYSIS TOOLS FOR IDENTIFYING THE PROPERTIES OF ACTIVE INGREDIENTS IN POLYMER COMPOSITIONS

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In this paper, a review of works using quantum-chemical methods and other mathematical modeling methods for the identification and control of the properties of polymer compositions is carried out. Some non-empirical methods are considered, as well as DFT methods and their role in modern research. The main stages of assessing the properties of polymer compositions are highlighted. Among them, the analysis of "structure-property," the control of the properties of polymer compositions both during polymerization and by varying active and passive additives. The main trends in the use of mathematical modeling for solving such problems are considered. The analysis of modern approaches used to study properties, among which neural networks and methods that require high-performance computing, is considered. Some of the models are described in detail, for example, the fundamental equations of the terminal model and the model of the penultimate unit. Examples also include the method of cellular automata, a mathematical model of the effect of an alternating electric field on a composite, the method of moments for calculating the average molecular weight, equations describing the polymerization process for high molecular weight compounds. This review also analyzed a new promising direction for using nanocomposites involved in the synthesis of new durable products with improved properties. The work carried out has shown that even at the same stages of assessing polymer compositions' properties, different quantum chemicals and other mathematical methods are used. The mathematical methods considered in this work can be systematized into three groups: modeling the structure-property relationship, controlling the properties during the synthesis of polymers, and controlling the properties of composite materials by changing the components of this composition.

Key words: quantum chemistry, mathematical modeling, composite materials, polymer compositions, nanocomposites

INTRODUCTION

Using quantum chemical and other computational chemistry methods to solve problems of identifying the properties of chemical structures has been topical in recent years. In terms of polymer structures, at first glance, it seems to a large extent theoretical and purely intellectual, but if we recall that the structural elements at any stage of the structure of a substance are inseparably linked with its properties, including technological and consumer, then the quantum chemical interest in such structures.

Nevertheless, in the modern problem-oriented scientific literature, it is still challenging to find their more or less attractive theoretical and applied terms, classification, subject analysis, and practical recommendations. Often, a different typology is introduced when describing methods in specific processes of a highly narrow purely synthetic laboratory orientation (for example, in the free polymerization of some monomers or in the radical polymerization [2, 42]) without any orientation towards promising experiments and practical goals.

In this review, an attempt is made to find practical results, generalize and classify quantum chemical methods of polymer chemistry, somewhat divorced from narrowly specific processes and conditions to highlight the vector of development of this field, including, perhaps, a distant connection with practice. We will once again emphasize that the use of high-molecular compounds (polymers) as a source and basis of modern broad-profile materials is determined by a complex of unique physical, mechanical and chemical properties, which, including in mixtures and composite products, are decisively a consequence of the chain structure of macromolecules, polymer matrices and structures formed by them, including composites.

As a traditional list of properties, one can cite high elastic moduli, flexibility, reversible deformations at high temperatures, interesting rheological characteristics, the ability to convert chemical energy into mechanical energy, and many more.

Now about polymer composite materials. Products made from them are widely used in industry and everyday life – from construction to radio engineering. Everyone knows that the most popular poly-

mer matrices, being individual or copolymer compounds, were synthesized in the last century, but even now, more and more new ones appear relatively often. In this regard, in our opinion, one of the essential tasks, especially for new objects, is the preliminary (presynthetic) determination of the properties of materialized chemical structures and the determination of their place in the developing set of IUDs of polymer materials.

Recall that most often, the solution of controlling the properties of polymeric materials occurs at different stages and today is carried out mainly experimentally, which often requires complex and long-term synthetic work, the use of expensive equipment, material costs, etc. In these conditions, no less critical are approaches that use computational chemistry to predict the properties of polymer and, more specifically, polymer composite materials [18, 22, 24, 40]: numerical methods, mathematical modeling, quantum chemical calculations, etc.

Speaking about quantum chemical calculations, we distinguish three large groups: ab initio methods; density functional theory (DFT) methods; and semiempirical methods.

Non-empirical methods (ab initio methods, from Lat. "From the beginning") are based on solving the original Schrödinger equation by successively applying simplifying approximations, the rigor of which is controlled, and the calculation formulas are deduced. In this way, rigorous design expressions are obtained to achieve a very high level of accuracy. These methods are of little use for polymer systems, therefore, this article is not considered in detail.

The density functional theory is based on the rejection of the use of the wave function to describe the system and the use of the electron density function for this purpose. As a result, the central equation is not the Schrödinger equation but its analog – the Kohn-Sham equations or other expressions.

DFT scope is vast – polymeric, organic, inorganic, organometallic, coordination and hydrogen-bonded compounds, molecular, crystalline, and amorphous.

An advantage over non-empirical methods is significantly higher productivity, making it possible to consider systems of a much larger size (by a factor of 10 or more) with an utterly comparable level of accuracy in reproducing structural, thermodynamic, electronic, and spectral parameters.

The advantage of DFT over semiempirical methods is the absence of the need to calibrate atomic parameters for a given type of atoms or a given class of systems and the stability of the results when passing to unknown classes of compounds [41]. Here it becomes possible to predict the properties. In the latter case, semiempirical methods often give nonphysical results since these compounds were not taken into account when calibrating semiempirical parameters.

In this part of this article, the leading modern approaches are given to design, predict and control material properties:

1. The "structure-properties" approach;
2. Management of properties during synthesis;
3. Management of properties of materials.

The levers for controlling the physicochemical and mechanical properties of polymers and polymeric materials at different stages of the latter's development are considered. In this part, we note in passing that the "structure-property" approach may not be based at all on a natural experiment, since the properties of an information object are studied according to specific characteristics of their constituent parts and initial conditions, the synthesis of polymers and the production of samples are assumed only to check the obtained best theoretical (calculated) results [25].

In chemistry and technology, a wide range of substances is used to obtain finished polymer products, including active and buffer additives, coatings, fillers, technological ingredients, etc. However, positive results are achieved in rather narrow directions by solving specific practical problems [4, 7, 12, 14, 15, 19, 20].

This approach, in comparison with others, is the most popular and is more significantly represented in modern scientific and technical literature; however, it was when working with the properties of finished materials within the framework of the structure-property relationship that we did not come across any preliminary calculations, modeling and calculations with practical results. For example, quantum chemistry methods are extremely rarely used in the analysis of the process of polymer synthesis, say, polymerization, when there is a sequential addition of molecules of one or several monomers to the growing active center of a macromolecule. Here, it seems, the use of this option for calculating the results of polymerization will give an active opportunity to control its conditions.

Let us give an example. Today, polymer nanocomposites – multicomponent materials consisting of a polymer matrix, fillers, and various other ingredients and nanoadditives – have gained widespread acceptance and popularity. All the constituent parts can interact with each other, and the systematic theoretical assessment of these interactions by mathematical methods in connection with the structure of the macromolecule and supramolecular formations becomes highly problematic. It is indicated, for example, by the study of a polymer composition with organomodified nanoclay [6]. Nanocomposites have improved properties as compared to conventional polymer systems.

Still, it is unlikely that their peculiarity can be predicted in advance, and the problem of identifying the properties of nanopolymer systems is now especially urgent and has good prospects shortly [10, 11, 13]. We tried to assess the capabilities of computational chemistry in this part as well.

Complex approaches to studying the properties of polymer composite materials as complex systems deserve significant attention. The researchers suggest the following route here – a preliminary consideration of the final material as a virtual object using suitable computational methods for analyzing the structure-property relationship (such a relationship does not need to exist for a particular object), analyzing the results, and selecting the best ones for a natural experiment, then computational support of the actual the process of polymer synthesis, and, finally, the assessment of synthetic results and the identification of the relationship between virtuality and reality. Then, in the case of a completely new object, a comprehensive study continues, followed by technical recommendations. However, we have not yet grown to such a level, although its vigorous shoots, as will be shown below, are found.

Even more rarely, one can find works related to mathematical and informational modeling of the interaction of chemical structures in the composition of several polymer matrices. Usually, one specific polymer is analyzed as a system, and the processes of interaction of monomers are discussed in connection with its synthesis. Here a wide field of activity arises, in which problem-oriented quantum-chemical methods can be nurtured, intended for the analysis of complex polymer systems, mainly consisting of several high-molecular compounds. The development of this direction can help in creating conditions for predicting the processes of interaction of structures within the system and manifestations of properties in the external environment, creating new objects, optimizing the composition, improving the conditions for synthesis and processing, and a more detailed study of the chemical properties of the system as a whole, etc.

ANALYSIS OF THE RELATIONSHIP "STRUCTURE – PROPERTIES"

Here we should note that quantum-mechanical calculations relate to quite specific polymer systems and specific indicators of properties, which lend themselves to the use of mathematics and computer technology and do not yet have a generalized and general methodological character. Let us summarize some of them. For example, a group of scientists [2] showed a relationship between the geometric structure and the optical and electrochemical properties of materials created from conjugated polymers and created a theoretical basis for developing original materials for various purposes. These studies established a relationship between the optical contrast of an electrically conducting polymer obtained by polymerization of 2,5-di(2-thienyl)-1H-pyrrole and the bandgap of the monomer. Besides, it was found that features in the geometric structure of the main chain of the molecule can cause a low charge density on the polymer itself. Thus, in this case, an approach to studying the essential physical properties of polymers has been determined, proceeding from the knowledge of the structure of the monomers that make up the macromolecule.

A similar approach was used in a study on the effect of the molecular structure of monomers on the mobility of the polymer chain [3], in which a set of dichalcogenides (disulfide and diselenide bonds) with different skeletons (PA, PD, and PF) in combination with five different functional groups as substituents has been studied using molecular dynamics modeling techniques. This simulation was carried out to reveal the dependence of the chain mobility and the role of hydrogen bonds in the theoretical consideration of the system's ability to restore. Derivatives of aromatic diselenides gave the best indicators.

Quite often in the scientific literature, an assessment of the properties of a polymer by the structure of the monomer of which it is composed is considered. There are both empirical and purely theoretical options. For example, a group of scientists [27] published a study evaluating the behavior of dispersed hydrophilic cellulose nanofibers (CNF) in hydrophobic isotactic polypropylene (iPP) using scattering and microscopy techniques to study fibers at the nanometer and micrometer scale, followed by theoretical analysis. The calculations of the properties were based on the empirical optical characteristics. The iPP composites reinforced with CNF fillers were characterized by small-angle light scattering, small-angle X-ray scattering, and molten material measurements using polarized optical microscopy. The shape of the CNF fillers and/or the larger aggregates formed from there was evaluated.

An approach that includes the study of the dynamics of changes in the structure of a substance and the effect of this change on properties can also be classified under the category of "structure-property" approaches. Such a dynamic effect is found, for example, in the study of the effect of cleaning fibers from carbon nanotubes (CNTs) on their mechanical and electrical properties and, more importantly, on the efficiency of various surface modifications. Even though cleaning mainly works on the surface of CNT fibers, the tensile

strength and electrical conductivity of CNT fibers increase from 0.50 N tex-1 and 932 S cm^{-1} to 0.91 N tex^{-1} and 5158 S cm^{-1} by restoring their defective structures and improving their alignment and density. Also, the efficiency of their surface modifications using covalent and non-covalent approaches is significantly increased. Au nanoparticles grow on cleaned CNT fibers much more densely than on spun CNT fibers. The obtained nanocomposite Au/CNT fibers demonstrate improved mechanical and physical properties, as well as the possibility of their use as a fibrous catalyst [28].

Other researchers have used one more version of the general method "structure-property" – fractional calculus. It was used to study the correlation between the complex modulus of elasticity and the complex relative permittivity of polystyrene (PS) film ~ 80 μm thick. Measurements were performed using dynamic mechanical analysis and dynamic dielectric analysis. Experimental results show mechanical and dielectric manifestations of essential relaxation (glass transition process), the molecular mobility of which has been analyzed using two innovative models: a fractional mechanical model and a fractional dielectric model. The parameters of fractional models show that with an increase in temperature, the molecular mobility, which is the basis of relaxation, also increases, but at the same time, the cooperativity of mobility decreases [29].

The technology of using neural networks in the search for relationships between the structures of chemical compounds and their properties has found wide application and development – the most commonly used feedforward multilayer neural network learning by the backpropagation method [35]. For polymers, the autoignition temperature [36], viscosity [37], and density [38] are most often studied. The generalized Widrow-Hoff delta rule and the flexible propagation method are also distinguished from the methods [39]. However, it is too early to conclude that the foundation has been laid.

POLYMER PROPERTY MANAGEMENT DURING SYNTHESIS

The development of computational methods and techniques aimed at studying the reactions of macromolecular processes associated with the addition of prominent radicals and taking into account the effect of chain length has led to the study of copolymer systems. They were first used in the early 2000s to study the copolymerization reaction. The first computational experiment in the analysis of a copolymer system was carried out in 2003 – the copolymerization of ethylene with vinyl acetate was investigated. As a result, the kinetics of all propagation reactions involved in its free polymerization process was characterized [1].

Many copolymer systems such as common acrylates and methacrylates, styrene and functional acrylates, and other typical monomers have been studied using the fundamental equations of the terminal model and the penultimate unit model [1]. In this case, such characteristics of monomers as the coefficient of propagation rate, coefficient of reactivity of monomers, activation energy, preexponential factor, etc. are used as initial data. They are presented below (1).

Terminal Model

$$\left.\begin{aligned} &RM_i^* + M_j \xrightarrow{k_{p,ij}} RM_iM_j^* \quad i,j = 1 \text{ or } 2 \\ &r_i = \frac{k_{p,ii}}{k_{p,ij}} \\ &F_i^{inst} = \frac{r_i f_i^2 + f_i f_j}{r_i f_i^2 + 2 f_i f_j + r_i f_j^2} \\ &k_{p,cop} = \frac{r_i f_i^2 + 2 f_i f_j + r_i f_j^2}{\left(\frac{r_i f_i}{k_{p,ii}}\right) + \left(\frac{r_j f_j}{k_{p,jj}}\right)} \end{aligned}\right\} \quad i \neq j \text{ and } i,j = 1 \text{ or } 2$$

Penultimate Unit Model

$$RM_iM_j^* + M_k \xrightarrow{k_{p,ijk}} RM_iM_jM_k^* \qquad i,j,k = 1 \text{ or } 2 \quad (1)$$

Determination of the ratios of reactivities and fundamental equations of the final and penultimate unit models of copolymerization of a binary system. RM_i^* – a radical with a terminal monomer unit of the type i; M_j – monomer type j; k – coefficient of propagation speed; r – coefficient of reactivity of monomers; F – instant copolymer composition; f – the composition of the monomeric phase; $RM_iM_j^*$ – a radical with a terminal monomer of the type j and the penultimate link of the type i; s – radical reactivity [1].

When solving the problems of controlling the processes of polymerization in solution, with a change in operating parameters, the most widespread approach is predicting the results of polymerization (degree of polymerization, yield, molecular weight distribution, etc.) in terms of quality indicators associated with the molecular characteristics of polymerization products. Note that at present, control over the molecular characteristics of polymers in actual technological processes is carried out in two main ways: directly by the measured molecular weight distribution (MWD) using gel permeation chromatography or by indirect parameters based on empirically obtained dependences [18]. In this approach, geometric indicators of molecules, rate constants of growth and chain transfer to a monomer, etc. are used as characteristics.

$$\left.\begin{aligned} r_i &= \frac{k_{p,iii}}{k_{p,iij}} \\ s_i &= \frac{k_{p,jii}}{k_{p,iii}} \\ r_i' &= \frac{k_{p,jii}}{k_{p,jij}} \\ \bar{r}_i &= r_i'\left(\frac{f_i r_i + f_j}{f_i r_i' + f_j}\right) \\ \bar{k}_{p,ii} &= k_{p,iii}\left(\frac{f_i r_i + f_j}{f_i r_i + \frac{f_j}{s_i}}\right) \\ F_i^{inst} &= \frac{\bar{r}_i f_i^2 + f_i f_j}{\bar{r}_i f_i^2 + 2 f_i f_j + \bar{r}_i f_j^2} \\ k_{p,cop} &= \frac{\bar{r}_i f_i^2 + 2 f_i f_j + \bar{r}_i f_j^2}{\left(\frac{\bar{r}_i f_i}{k_{p,ii}}\right) + \left(\frac{\bar{r}_j f_j}{k_{p,jj}}\right)} \end{aligned}\right\} \quad i \neq j \text{ and } i,j = 1 \text{ or } 2$$

It shows, in particular, a study on mathematical modeling of the synthesis of diene rubber on a neodymium-containing catalytic system for a cascade of continuous reactors. The influence of operating parameters on the molecular weight characteristics and physicomechanical properties of the synthesized polymer was investigated using the molecular weight distribution [18]. The model is described by equations (2), (3).

Differential equations for the concentration of monomer and macromolecules in the i-th reactor of the cascade contain terms that describe the growth of macromolecules and a gradual increase in their length and changes in their number of active centers. Equations (3) are written for a steady-state polymerization process in the long-chain approximation used for high molecular weight compounds [18].

In equations (3), $R_k(i,l)$ are the concentration of i macromolecules with active centers and l monomeric units in the ith reactor of the cascade; $k_{p\,k}, k_{tm\,k}, k_{tp\,k}, k_{Al\,k}, k_{sp\,k}$ are the rate constants of growth, chain transfer to a monomer, polymer, organoaluminum compound, and spontaneous chain transfer, respectively; δ_{ij} is the Kronecker symbol, $\delta(l)$ is the generalized Dirac function [18].

$$\frac{M_{k-1} - M_k}{\tau} - k_{p\,k} M_k I_0 = 0, \qquad k = 1,2,3 \ldots$$
$$\frac{A_{k-1} - A_k}{\tau} - k_{tAk} A_k I_0 = 0 \qquad (2)$$

$$\begin{aligned} &\frac{R_{k-1}(i,l) - R_k(i,l)}{\tau} - ik_{pk} M_k \frac{\partial R_k(i,l)}{\partial l} + \\ &+ k_{tp\,k} l I_0 [R_k(i-1,l) - R_k(i,l)] + \\ &+ \left(k_{tp\,k}(M_0 - M_k) + k_{sp\,k} + k_{tm\,k} M_k + k_{tAk} A_k\right) \times \\ &\times [(i+1)R_k(i+1,l) - iR_k(i,l)] + \\ &+ \frac{I_0}{\tau}\delta_{k\,1}\delta_{i1}\delta(l) + \\ &+ \left(k_{sp\,k} + k_{tm\,k} M_k + k_{tAk} A_k\right) I_0 \delta_{i1}\delta(l) = 0, \\ &0 \le l < \infty, i = 0,1,2 \ldots \end{aligned} \qquad (3)$$

The dielectric properties of polymer-ceramic composite materials were also described by the method of asymptotic averaging, using mathematical modeling [22]. The description of the effect of an electromagnetic field on highly inhomogeneous media is carried out using equations with rapidly oscillating coefficients characterizing the properties of individual components of the composite material. The main idea of the method of asymptotic averaging of differential equations (MAO), proposed by NS Bakhvalov and A. Bensussan [32-34], consists of replacing a heterogeneous material with a homogeneous medium with averaged physical and mechanical parameters. An MAO modernization has been developed to calculate the effective properties of complexly structured composite materials with the property of central symmetry, which brings the problem with periodic boundary conditions to a series of problems solved with adapted components in the directions of space to establish the practical characteristics of the composite and the dielectric loss tangent [24]. A mathematical model of an alternating electric field effect on a composite is given below (4).

$$\left\{\begin{array}{ll} D_{i/i}^{*\alpha(0)} = 0, & x_i \in V_{\xi\alpha} \\ D_i^{*\alpha(0)} = \varepsilon^{*\alpha} E_i^{*\alpha(0)}, & x_i \in V_{\xi\alpha} \\ E_i^{*\alpha(0)} = \overline{E_i^*} + \varphi_i^{*\alpha(1)}, & x_i \in V_{\xi\alpha} \\ \varphi^{*\alpha(1)} = \varphi^{*N(1)}, \left(D_i^{*\alpha(0)} - D_i^{*N(0)}\right) n_i = 0, & x_i \in \Sigma_{\xi\alpha N} \\ < \varphi^{*\alpha(1)} > = 0, \left[\left[D_i^{*(0)}\right]\right] n_i = 0, \left[\left[\varphi^{*\alpha(1)}\right]\right] = 0, & x_i \in \Sigma_{\xi\alpha N} \end{array}\right\} \qquad (4)$$

where $< \varphi^{*(1)} >$ – averaging operation over the "periodicity cell", $\left[\varphi^{*(1)}\right]$ – periodicity conditions, $\overline{E_i^*}$ – average tension of the composite.

Sometimes, using mathematical modeling tools, polymerization conditions are selected. For example, in one of the works, based on a mathematical model, the dependence of the values of the monomer concentrations on the polymerization time was constructed, and the values of the number-average and weight-average molecular weights were also found [24]. In this case, the constants of the elementary stages of initiation, chain growth, chain transfer to the monomer, and deactivation were used in the calculations. The average molecular weights of the polymer were calculated by the method of moments (5).

$$\frac{d[I]}{dt} = -k_i[I],$$

$$\frac{d[P_0]}{dt} = fk_i[P_0] - k_p[M][P_0],$$

$$\frac{d[P_1]}{dt} = -k_p[M][P_0] + k_m[M]\mu_0 + k_\alpha[A]\mu_0 - -k_d[P_1],$$

$$\frac{d[M]}{dt} = -(k_p + k_m)[M][P_1] - (k_p + k_m)[M]\mu_0, \quad (5)$$

$$\frac{d[Q_1]}{dt} = k_m[M][P_1] + k_\alpha[A][P_1] + k_d[P_1],$$

$$\frac{d[A]}{dt} = -k_\alpha[A][P_1] - k_\alpha[A]\mu_0,$$

$$\frac{d\mu_0}{dt} = \sum_{i=2}^{\infty} \frac{d[P_i]}{dt} = k_p[M][P_0] - -(k_m[M] + k_\alpha[A] + k_d)\mu_0,$$

$$\frac{d\mu_1}{dt} = \sum_{i=2}^{\infty} i\frac{d[P_i]}{dt} = (1 + \mu_0)k_p[M][P_0] \cdot \cdot(k_m[M] + k_\alpha[A] + k_d)\mu_1,$$

$$\frac{d\mu_2}{dt} = \sum_{i=2}^{\infty} i^2\frac{d[P_i]}{dt} = (\mu_2 + 2\mu_1 + \mu_0)k_p[M][P_0] - -(k_p[M] - k_m[M] + k_\alpha[A] + k_d)\mu_2,$$

$$\frac{d\eta_0}{dt} = \sum_{i=2}^{\infty} \frac{d[Q_i]}{dt} = (k_m[M] + k_\alpha[A] + k_d)\mu_0.$$

where M – monomer molecules, A – organoaluminum compound, I – initiator molecules, P_n, Q_n – active and inactive polymer chains of length i, respectively, the content of i units M of the monomer, k_i, k_p, k_m, k_a, k_d – constants of the elementary stages of initiation, chain growth, chain transfer to a monomer, to an organoaluminum compound, and deactivation of active centers, respectively.

MANAGEMENT OF PROPERTIES OF FINISHED POLYMERS

Currently, a method for controlling the properties of finished polymers by introducing various additives is widely used. The most common task here is the task of controlling the physicomechanical properties of polymers. It is still a complex problem to add, for example, to a rubber compound this kind of filler (without other additives), which will make it possible to obtain a solid but rigid product using an elastomer as a polymer matrix. There are many approaches to solving such problems. For example, with the biometric design of graphene oxide-coated polyurethane rubber, the tensile strength and elongation at break have been improved, and the maximum decomposition temperature of the material has been increased [12]. Another experiment was performed with reduced graphene oxide. The mechanical properties of the material, particularly the modulus of elasticity and the modulus of storage, were improved by adding two metallic particles (boron and nickel). Preliminary calculations were carried out using atomistic modeling [14].

In addition to alloying of polymers, reinforcement is often found to improve the properties of a material. As an example, wollastonite, which is gaining popularity in recent years, is a functional filler with great potential for use in thermoplastic composites, replacing more expensive reinforcement such as fiberglass. In addition to the price advantage, wollastonite has a high aspect ratio and hardness and can also improve the tensile and flexural strength of polymer composites [15]. Here, a preliminary estimate of the potential properties greatly facilitates the search algorithm.

Often, a new composite is synthesized for specific goals and objectives of forecasting. For example, one of the work reports shows developing a flexible conductive composite with carbon black as an effective electrode material for replacing graphite in the electrochemical synthesis of supercapacitive polyaniline (PAni). The new composite showed high volumetric electrical conductivity and concentration of charge carriers in combination with good mechanical properties, which coincides with analytics [7].

In addition to physical and mechanical properties, the chemical and biological parameters of polymeric materials and forecasts in this part are often of interest. In one of the works of Turkish specialists, the influence of the content of short carbon fiber (SCF) and hydroxyapatite (HAp) on the mechanical, tribological, and biological properties of the composite was studied [4]. In another study, a harmful pressure stirring method was used to prepare a homogeneous graphene-based polydimethylsiloxane composite (PDMS). This method was used for the first time and helped solve graphene agglomeration in a polymer matrix using aerogels of graphene microspheres. They have a unique porous structure and excellent adsorption capacity, allowing the PDMS solution to uniformly fill reduced graphene oxide airgel (rGOAM) airgel microspheres or GO airgel microspheres (GOAM) under reduced pressure [8]. Graphene oxide is very popular with scientists today. As the forecast and some practical achievements show, it can be used to control the electrically conductive properties of hybrids based on lactic acid and thermoplastic starch [9].

One of the popular areas of theoretical analysis in quantum chemistry is nanocomposites. Recall that polymer nanocomposites are materials containing nanosized inclusions in polymer matrices [26]. It is

known here that the result of the addition of nanoparticles of fibers is a dramatic improvement in a set of functional properties, which may include mechanical, electrical, thermal, acoustic, etc.

Polymer nanocomposites have generated tremendous interest in recent years to develop high-performance products such as lightweight sensors, thin-film capacitors, batteries, flame retardant products, biodegradable and biocompatible materials, etc. For the past several decades, the field of polymer nanocomposites has been at the forefront of polymer research. Moreover, a vast number of studies have been published.

Here, as indicated above, active additives are also one of the main tools for controlling the properties of nanocomposites. It would be helpful to expand the possibilities of the theory here – the results can be auspicious. Let us note some. For example, a series of framework siloxanes (spherosilicate [SS] type) have been tested as functional additives to obtain nanocomposites based on polyethylene (PE) [6]. Rheological, mechanical, and thermal properties were studied. The results were compared with similar reports for polyethylene systems reinforced with silsesquioxane and SS. It turned out that the use of nanocomposites significantly improves the above properties. It is confirmed in the following experiment: a significant improvement in the electrical conductivity of polyetherimide (PEI) foams filled with graphene nanoplates was achieved by simultaneously increasing the porosity and dispersion of graphene nanoplates. Foams were prepared by phase separation induced by water vapor using graphene nanoplates (GNPs) with a concentration of 1 to 10 wt%. [10] Separate properties of a particular nanocomposite are also being studied. A group of scientists investigated the optical and dielectric properties of the initial nanocomposite based on incorporating carbon dots (C-dots) into polymethyl methacrylate (PMMA) with several filler loads. [11] Hybrid silica/montmorillonite nanoparticles were prepared to modify high-density polyethylene used to make wood/polymer composites (WPC). With their help, higher mechanical strength and interfacial compatibility between wood and polymer were achieved [13].

Here, mathematical modeling is often used to calculate the properties of nanocomposites. For example, the process of deformation of nanocomposites was calculated by the method of cellular automata. Two parallel calculations were carried out in two blocks of calculations, in which indicators of the geometric structure of molecules are used. They are indicated in the formulas below [23]:

Block of the first type:

Calculation of the force acting on the cell

$$F_{ik}^{x} = \sigma^{x} S;\ F_{ik}^{y} = \sigma^{y} S;\ F_{ik}^{z} = \sigma^{z} S \quad (6)$$

Cell elongation calculation

$$\Delta l_{ik}^{x} = \frac{l_0 \sigma^{x}}{E_{ik}};\ \Delta l_{ik}^{y} = \frac{l_0 \sigma^{y}}{E_{ik}};\ \Delta l_{ik}^{z} = \frac{l_0 \sigma^{z}}{E_{ik}} \quad (7)$$

Calculation of the resulting force acting on the cell along the X, Y, Z axes

$$\begin{aligned} F_{p,kx}^{x} &= F_{i,k}^{x} \pm F_{i-1,k}^{x} \pm F_{i+1,k}^{x} \pm F_{i,k-1}^{x} \pm F_{i,k+1}^{x}, \\ F_{p,ky}^{y} &= F_{i,k}^{y} \pm F_{i-1,k}^{y} \pm F_{i+1,k}^{y} \pm F_{i,k-1}^{y} \pm F_{i,k+1}^{y}, \\ F_{p,kz}^{z} &= F_{i,k}^{z} \pm F_{i-1,k}^{z} \pm F_{i+1,k}^{z} \pm F_{i,k-1}^{z} \pm F_{i,k+1}^{z}, \end{aligned} \quad (8)$$

Calculation of the resulting elongation

$$\Delta l_{p,ik}^{x} = \frac{F_p^{x}}{E_{ik} l_0};\ \Delta l_{p,ik}^{y} = \frac{F_p^{y}}{E_{ik} l_0};\ \Delta l_{p,ik}^{z} = \frac{F_p^{z}}{E_{ik} l_0}; \quad (9)$$

Block of the second type:

Calculation of effective elongation

$$\Delta l_{pi,k}^{x} = \frac{\sum_{j=1}^{n_j} \sum_{k=1}^{n_k} \sum_{i=1}^{n_i} \Delta l_{pi\,j\,k}^{x}}{n_k n_i};\ \Delta l_{pi,k}^{y} = \frac{\sum_{j=1}^{n_j} \sum_{k=1}^{n_k} \sum_{i=1}^{n_i} \Delta l_{pi\,j\,k}^{y}}{n_k n_i};\ \Delta l_{pi,k}^{z} = \frac{\sum_{j=1}^{n_j} \sum_{k=1}^{n_k} \sum_{i=1}^{n_i} \Delta l_{pi\,j\,k}^{z}}{n_k n_i} \quad (10)$$

Calculation of the effective modulus of elasticity of compression

$$E_{эфф} = \frac{n_k n_j n_i \sigma l_0}{\sum_{k=1}^{nk} \sum_{j=1}^{nj} \sum_{i=1}^{ni} \Delta l_{p,kji}} \quad (11)$$

Another option for calculations is the effect of passive additives and coatings on polymer properties. For example, Epoxy Asphalt Bond Coating (EABC) is widely used as a tie coat in orthotropic steel bridges. To withstand the vibration of the steel deck, the EABC must have a high bond strength. An experiment was designed and conducted where sodium montmorillonite (Mt) was used to enhance pure EABC. The morphology and properties of EABC/Mt nanocomposites were characterized using scanning electron microscopy, X-ray diffraction, Brookfield rotary viscometer, dynamic mechanical analysis, thermogravimetric analysis, automatic adhesion tester, and universal testing machine. The inclusion of Mt increased the viscosity of pure EABC at the initial stage of the chemical reaction and also slightly lowered the glass transition temperature of pure EABC. The addition of Mt significantly improved the mechanical properties of pure EABC and increased its adhesive strength [16].

CONCLUSION

Thus, the preceding shows that the use of mathematical models and methods of quantum chemistry in the field of analysis of polymer structures has a theoretical and practical basis and makes it possible to

predict various properties of the polymer both during synthesis (time and conditions of polymerization) and the structure during the production of the material, including both complex and straightforward options; and interactions with additives and fillers. Often, calculations are accompanied by a natural experiment, which immediately shows the relevance and accuracy of the model or method. However, in many cases, it is not yet possible to test the theory empirically due to the high cost of equipment, complexity, energy consumption of processes, its long periods, etc. However, there is progress in this direction.

It will not be superfluous to note once again the specificity of our time – today, polymers are an integral component of a wide range of promising nanocomposites and hybrid nanomaterials. Further development of the scientific and technological principles of nanophysics, nanochemistry, nanotechnology in general, and mathematical and information methods opens up great opportunities for expanding the areas of the practical application of polymer systems and provide material for theoretical analysis. Therefore, as this review shows, studies of nanocomposites and nanomaterials turned out to be more thoroughly developed and widely represented in the modern scientific literature. The authors of the articles themselves explain this by synthesizing high-performance, technologically advanced, durable products.

Because of the wide variability of the polymers themselves and their properties, it is rather challenging to identify a single system for determining the best method or the most suitable model for a certain kind of problem. Even in similar theoretical approaches of the "structure-property" type, completely different models and methods are used.

Thus, any systematization, or classification, is helpful in this area of research. The study of polymers using mathematical modeling and quantum chemistry methods, as indicated in the review, has made some progress in specific directions. For example, the copolymerization process is most often described by the fundamental equations of the terminal model and the model of the penultimate unit [1, 30, 31]. A significant role in this is played by the use of high-performance computing, for example, using the method of cellular automata [23].

The authors declare the absence a conflict of interest warranting disclosure in this article.

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