Mathematical methods for predicting the durability of polymer composites under extreme conditions

Evgeny Gusev[1,2,*], *Vladimir* Bakulin[3], and *Vera* Chernykh[1,2]

[1]Institute of the problems to Oils and Gas of Research Scientific Center "Yakut Scientific Center of the Siberian Branch RAS", 2, Petrovskogo st., Yakutsk, 677980, Russia
[2]Institute of Mathematics and Informatics, North-East Federal University, 48, Kulakovskogo st., Yakutsk, 677000, Russia
[3]Institute of Applied Mechanics of Russian Academy of Sciences, 7, Leningradsky prospekt, Moscow, 125040, Russia

Abstract. The paper investigates the issue of promising ways to predict the durability of polymer composites under extreme conditions. A study of the possibility of predicting the durability of the material, based on the information obtained in the first years of operation. Based on the modern provisions of molecular kinetic theory (MKT), the issue of matching the defining parameters of mathematical models calculated because of solving forecasting problems within the framework of the formulated variational formulation, considering the results of experimental measurements at the macro level, with the corresponding defining parameters of physical models describing molecular interactions at the micro-level, was investigated. The results of computational experiments are presented.

1 Introduction

In recent decades, increasing attention has been paid to the problem of creating reliable methods for quantifying the performance of products made of polymer and composite materials [1–3]. The importance of developing effective high-precision methods for long-term forecasting of the defining characteristics of composites (residual life, strength, reliability, durability) is since composite materials and structures made of them are an integral part of modern technology in such areas that determine scientific and technological progress as aviation and space technology, shipbuilding, oil, and gas industry, etc. [2–4].

Currently, the problems of mathematical modeling of problems of long-term forecasting of the durability of structures made of polymer composites under extreme conditions, under the influence of extreme climatic environmental factors, are solved in significantly simplified formulations that do not consider a significant number of factors that have a significant impact on the accuracy of the solution. As a rule, the applied forecasting models have a small number of uncertain parameters, which does not allow achieving the necessary degree of adequacy of the model of the real situation. At the same time, an integral part of the problem of developing effective methods for predicting the defining characteristics of composites is solving the problem of effectively constructing globally optimal solutions that evaluate the effectiveness of the constructed solutions to forecasting problems.

*e-mail: elgusev@mail.ru

The specificity of the studied problems of predicting the defining characteristics of polymer composite materials (PCM) under extreme conditions leads to the fact that for these problems the extrapolation approach in the traditional formulation is ineffective. As noted in several papers [5–8], a fundamental improvement of the extrapolation approach can be achieved based on the choice of a mathematical model with a focus on physical representations. The paper investigates the prospects of predicting the durability of polymer composites in extreme conditions. A study of the possibility of predicting the durability of materials, based on the information obtained in the first years of operation.

2 Application of the basic provisions of the molecular kinetic theory for the construction of generalized durability models

The development of generalized models of the durability of composites under extreme conditions is based on the main provisions of the modern molecular kinetic theory (MKT). This is because chemical transformations in composites can occur both at intermolecular and intramolecular levels.

It is known from the Boltzmann distribution for the kinetic energy of molecules that the number of molecules with energy E greater than the activation energy E_a is proportional to the exponent $\exp(-E_a/RT)$. As a result, the rate of a chemical reaction is represented by the Arrhenius equation obtained from thermodynamic considerations, which has the form in functional and differential forms:

$$k = k_0 \exp(-E_a/RT), \quad d(\ln k)/dT = E_a/RT^2. \tag{1}$$

Analysis of the Arrhenius equation (1) in differential form shows that the greater the activation energy E_a, the faster the reaction rate constant k increases with increasing temperature. In these notations, R is the Boltzmann constant. The frequency factor k_0 characterizes the collision frequency of reacting molecules (the number of active collisions of particles per unit volume in the reaction mixture). The frequency factor k_0 expresses the fraction of particles whose energy is equal to or greater than the activation energy E_a. The activation energy E_a is an excess of energy relative to the average energy of the particles at a given temperature, which is necessary for the reacting particles to enter a chemical reaction and is determined by the properties of the reacting particles, their energy state.

Following the main provisions of the MKT, the study was based on a physical model in which the nature of the change in time of the determining property of the composite R under the simultaneous influence of several extreme factors is determined by elementary chemical reactions at the molecular level described by the superposition of Arrhenius equations describing various types of molecular interactions initiated by the influence of various extreme factors $F_1, F_2, \ldots, F_p$ on the composite.

If various physical factors have an impact on the polymer composite, independent of the impact of other factors, and the changes caused in the composite are summed up, it can be assumed that a generalized durability model describing the simultaneous impact of several factors can be represented as:

$$R = R_0 + \sum_{j=1}^{p} F_j(u_{j,1}, u_{j,2}, \ldots, u_{j,l_j}; t). \tag{2}$$

By the current provisions of the MKT, it was assumed that the effect of each of the F_j factors on the composite activates at the micro-level a set of destructive elementary processes, the chemical reactions occurring in which can be described in the form of a superposition of Arrhenius equations. Each of the Arrhenius equations that make up the superposition

describes a certain type of elementary chemical reaction, with its inherent parameters—the frequency factor characterizing the frequency of collisions of reacting molecules, and the activation energy.

3 Variational formulation of forecasting problems of defining characteristics of composites

Following the formulated provisions of the MKT, each factor F_j can be represented as a superposition of the Arrhenius equations in the following form:

$$F_j(u_{j,1},\ldots,u_{j,l_j};t)=\sum_{k-1}^{N_j}\alpha_{kj}(u_{j,1},\ldots,u_{j,l_j})\left[\exp\left(\beta_{kj}(u_{j,1},\ldots,u_{j,l_j})t\right)-1\right],$$
$$j=1,2,\ldots,p;\quad 0\le t\le T_{\max}. \tag{3}$$

N_j is the number of elementary destructive processes, the course of chemical reactions in which is activated when the j-th factor is exposed to the composite, $u_{j_1},u_{j_2},\ldots,u_{j,l_j}$—parameters describing the nature of the impact of the j-th factor on the composite.

The parameters $\alpha_{kj}=\alpha_{kj}(u_{j_1},u_{j_2},\ldots,u_{j,l_j})$ express the fraction of particles whose energy is greater than or equal to the activation energy required to initiate the k-th elementary chemical reaction ($k=1,2,\ldots,N_j$) when exposed to the composite factor F_j; the parameters $\beta_{kj}=\beta_{kj}(u_{j_1},u_{j_2},\ldots,u_{j,l_j})$ are related to the activation energy, i.e. with an excess of energy relative to the average energy of the particles at a given temperature, necessary for reacting particles to initiate the k-th elementary chemical reaction ($k=1,2,\ldots,N_j$) when exposed to the composite factor F_j. The excess energy associated with the activation energy is determined by the properties of the reacting particles, their energy state.

Variational formulation of forecasting problems of defining characteristics of composites: Based on short-term tests conducted on the time interval of retrospection $[0,T_{\min}]$, it is necessary to find optimal parameters $u_1^*,u_2^*,\ldots,u_n^*$ of a generalized durability model $R(u^*;t)$ that deliver a global minimum to the efficiency criterion (4) on a set of multiparametric generalized forecasting models $\{R(u;t)\}$ that allow forecasting with an error not exceeding the predetermined maximum permissible error of the forecast $\gamma_R^{\max}$ (5):

$$\tilde{S}=S(u,Q)=\frac{1}{m}\sum_{i=1}^{m}\left[R(u_1,u_2,\ldots,u_m;t)-\tilde{R}_i\right]^2\Rightarrow\min_{u\in U}, \tag{4}$$

$$\max_{T_{\min}\le t\le T_{\max}}\left|\tilde{R}(t)-R^*(t)\right|\le\gamma_R^{\max}. \tag{5}$$

In these notations: $\tilde{R}_i=R_i(Q)$—measured values of the defining characteristic R at time points $t_1,t_2,\ldots,t_m$, considering measurement errors $Q_1,Q_2,\ldots,Q_m$. $R^*(t)$ real-time dependence. Vector of undefined parameters $u^*(Q)$ delivers the global minimum of the total standard error $\tilde{S}$ (4):

$$S(u^*(Q);Q)=\min_{u\in U}S(u;Q). \tag{6}$$

4 Problems of matching mathematical parameters and physical models within the framework of the formulated variational statement

Based on the modern provisions of the molecular kinetic theory, the question of matching the defining parameters of mathematical models calculated because of solving forecasting problems within the framework of the formulated variational formulation, considering the results of experimental measurements at the macro level, with the corresponding defining parameters of physical models describing molecular interactions at the micro-level, was investigated.

Several fundamental principles and concepts were introduced that allow for optimal coordination of the defining parameters calculated based on the constructed mathematical models at the macro level with the defining parameters of physical models describing molecular interactions at the micro-level.

Such concepts and principles as the principle of a multiplicity of forecasting models, forecasting models of optimal structure and complexity, maximum permissible accuracy of the forecast, etc. are introduced. Within the framework of the formulated variational statements of forecasting problems, a parametric family of generalized durability models $\{R^N(;t)\}$, $(1 \le N < \infty)$ has been studied, in which the parameter is the number of terms N in the decomposition of the durability function into a series. Within the framework of the introduced parametric family of generalized durability models $\{R^N\}_{N=1}^{\infty}$, a forecasting model of optimal structure and complexity is constructed, which is understood as a model containing the optimal number of terms that allows solving the forecasting problem with the required accuracy.

The problem of constructing a model of optimal structure and complexity is reduced to solving the following extreme problem:

$$\max_{T_{\min}\le t\le T_{\max}} \left|R^{N^*}(u^{*N^*};t) - R^*(t)\right| = \min_{1\le N<\infty} \max_{T_{\min}\le t\le T_{\max}} \left|R^N(u^{*N};t) - R^*(t)\right|,$$
$$\max_{T_{\min}\le t\le T_{\max}} \left|R^N(u^{*N};t) - R^*(t)\right| \le \gamma_{\max}, \quad 1 \le N < \infty. \tag{7}$$

In these notations, $N^*$is the optimal number of parameters of the prediction model of optimal structure and complexity R^{N^*}; u^{*N}—the optimal vector of parameters of the optimal forecasting model of the parametric family corresponding to the parameter N; $\gamma_{\max}$—the maximum allowable error in solving the prediction problem.

By the principle of the multiplicity of forecasting models, it is considered that if in each multiparametric family of generalized forecasting models there is a model that is most adequate to the real predicted time dependence $R^*(t)$, then this model in the considered parametric family is a model of optimal structure and complexity.

The physical problems of restoring the parameters of destructive chemical reactions initiated by the action of extreme environmental factors are formulated in mathematical form within the framework of refined variational formulations of inverse problems of predicting the defining characteristics of PCM. Following the formulated principle of the multiplicity of forecasting models and the introduced concept of optimal forecasting models of optimal structure and complexity in the variational model [9–11], the task of restoring uncertain parameters can be reduced to finding the global minimum of the functional J, assessing the degree of adequacy of the model describing the impact of extreme environmental factors on the composite

$$J\left(\left\{\left(u^*_{j,1}, u^*_{j,2}, \ldots, u^*_{j,l_j}\right)\right\}_{j=1}^{p}\right) = \min_{\{u_{jk}\}} J\left(\left\{\left(u_{j,1}, u_{j,2}, \ldots, u_{j,l_j}\right)\right\}_{j=1}^{p}\right). \tag{8}$$

To construct the global minimum in the extreme problem (8), combined methods of searching for the global extremum have been developed, based on the combined application of necessary and sufficient conditions of the extremum and methods of full search.

5 Results of computational experiments based on generalized durability models

Figure 1 shows the results of computational experiments on predicting the residual life of polymer fiber composites (PFC) within the framework of the developed methodology. The simultaneous effect of two factors was considered: the hardening factor and the aging factor.

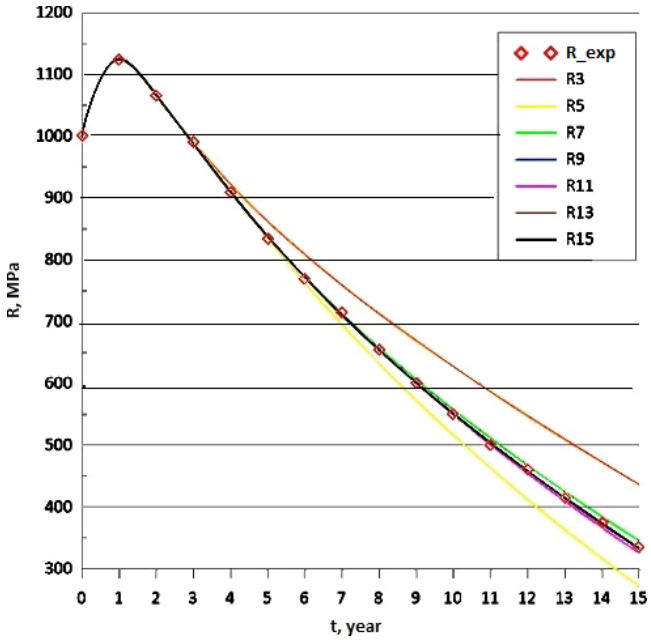

Figure 1. Optimal durability functions constructed based on optimal generalized forecasting models for retrospection intervals, the sizes of which are sequentially 3, 5, 7, 9, 11, and 13 years

As initial data for the construction of generalized models of the durability of the optimal structure and complexity based on the Arrhenius equations, the results of physical experiments on measuring the residual life of PFC were used.

Based on the computational experiments carried out according to the developed methodology, optimal multiparametric generalized models of the durability of the optimal structure and complexity were constructed with a sequential increase in the size of the time interval of retrospection.

The graph shows simultaneously all the optimal durability functions calculated based on the developed methodology, respectively, for the retrospection intervals, the sizes of which are sequentially 3, 5, 7, 9, 11, and 13 years. Experimental values are marked with diamonds on the graph. In the given designations: R3—forecast of the residual resource according to the data for the first 3 years of exposure, R5—according to the data for the first 5 years, etc.

Conducting computational experiments based on the developed methodology can help achieve a balance between exposure time and the accuracy of the forecast results.

6 Conclusion

The developed methodology for matching the parameters of mathematical and physical models at the micro and macro levels allowed solving the problem of restoring the parameters of physics-chemical processes occurring at the molecular level and leading to destructive changes in composites and deterioration of their characteristics over time.

An objective assessment of the parameters of destructive elementary chemical reactions in composites based on the conducted physical experiments made it possible to build effective generalized forecasting models for the long term, to conduct a constructive analysis of the influence of individual extreme factors on the durability of the composite, to give a comparative

assessment of the degree of influence of one or another extreme factor on the durability of the composite. Knowledge of the parameters of destructive elementary chemical reactions in the composite initiated by the action of extreme environmental factors, their comparative constructive analysis, can allow us to develop a methodology for the synthesis of new materials with increased durability.

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References

[1] A.Y. Bashkarev, V.I. Vettegren, M.A. Suslov, *Longevity polymeric composites* (Publishing House of Saint Petersburg Polytechnic University, Saint Petersburg, 2016)

[3] A.I. Reutov, *Forecasting to climatic stability polymeric materials, applicable in construction*, Vestnik Tomskogo gosudarstvennogo architecturno-stroitelnogo universiteta, **2**, 127 (2009)

[3] S.A. Lurie, Yu.O. Solyaev, D.Q. Nguen et al., *Composites: Mechanics, Computations, Applications: An International Journal*, **3**, 1 (2015)

[4] A.M. Dumansky, L.P. Tairova, *Time-dependent behavior of carbon fiber reinforced laminates*, in Proceedings of the Second Int. Conference on Advanced Composite Materials and Technologies for Aerospace Applications, 11–13 June 2012, Wrexham, North Wales, United Kingdom, 75 (2012)

[5] U.S. Urzhumtsev, I.N. Chersky, *Scientific foundations of engineering climatology of polymer and composite materials*, Mechanics of Composite Materials, **4**, 708 (1985)

[6] V.N. Bulmanis, V.A. Yartsev, V.V. Krivonos, *Efficiency design from polymeric composites at influence of the steady-state loads and climatic factors*, Mechanics of Composite Materials, **5**, 915 (1987)

[7] O.N. Karpuhin, *Determining the service life of a polymer material as a physics-chemical problem*, Uspehi himii, **8**, 1523 (1980)

[8] I.S. Filatov, R.N. Bochkarev, *Some problems of assessment and forecasting of climatic stability of polymer materials*, Methods for assessing climatic stability of polymer materials, 11 (YF AN SSSR, Yakutsk, 1986)

[9] E.L. Gusev, V.N. Bakulin, *Variation formulations of inverse problems in forecasting the residual life of composites*, Doklady physics, **63**, 388 (2018)

[10] E.L. Gusev, *Using parallel procedures for the searching of the extremum for the decision of the inverse problems prediction of the defining characteristics of the composite materials*, Material Physics and Mechanics, **26**, 70 (2016)

[11] E.L. Gusev, V.N. Bakulin, *Optimal control under a decrease in the thermal-field intensity based on selection of the heterogeneous-construction structure in the variational formulation*, Doklady physics, **63**, 213 (2018)