Analytical Description of the Kinetic Processes of Forming the Properties of Composites

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Abstract. Effective methods are proposed for approximating the kinetic processes of formation of physical and mechanical characteristics of composite materials for solving problems of both single-criterion and multi-criteria optimization of their structure and properties. The approximation of kinetic processes on a given interval with the definition of partial intervals of the maximum length approximation is considered in detail. An approximation algorithm on cubic splines is given. To determine the transfer functions of composites, as dynamic systems with many inputs and outputs, it is recommended to use Laguerre polynomials. The possibility of a cognitive approach is also not excluded with the direct selection of the form of the approximating function.

1. Introduction
The development of new composite materials with a regulated structure and properties is directly related to the analytical description of the kinetic processes of the formation of their physico-mechanical characteristics.

Often the process of formation of the operational value of the parameter (property) has an exponential aperiodic character (Fig. 1).

![Figure 1. Aperiodic kinetic process.](image)

2. An approximation algorithm with the maximum length of partial
Among a number of methods of approximation of these processes the special place owing to his simplicity is occupied by piecewise and linear approximation, as a rule, on sites of identical length. However, in many cases it is advisable to break down the kinetic processes into separate sections,
based on ensuring the maximum length of the approximation sections. As parameters of kinetic processes, various characteristics can be used that integrally determine the processes of formation of properties [1-4].

Data input. Specifies interval $[a, b]$, the relative error of approximation $\varepsilon_0$ in percent. Function $f(x)$ is realized as a program for calculating its values at any point $x \in [a, b]$ or at least at points $x_j, j = 0, N; x_0 = a, x_N = b$ such that $|f_j - f_{j+1}| \leq \frac{2\varepsilon_0}{1000}, f_{cp} = \frac{1}{N} \sum_{j=1}^{N} |f_j|, f_j = f(x_j)$.

The implementation of the algorithm was carried out according to tabular values of $(x_j, f_j)_{j=0}^{N}$ for an absolute error of $\varepsilon = \frac{\varepsilon_0}{100} \frac{1}{N} \sum_{j=1}^{N} |f_j|$ with a tabulation density of $|f_j - f_{j+1}| \leq 0.2\varepsilon$.

Tabulation. Here the program for obtaining information is implemented. The following algorithm was used. For $h = 0.04(b-a), N = \frac{b-a}{h}$ we compute:

$$x_j = a + jh, \quad f_j = f(x_j), j = 0, N; \quad \varepsilon_h = \max_{1 \leq j \leq N} |f_j - f_{j+1}|; \quad f_{cp} = \frac{1}{N} \sum_{j=1}^{N} |f_j|, \quad \varepsilon = \frac{\varepsilon_0}{100} f_{cp}.$$  

At $\varepsilon_h > 0.2\varepsilon$ the value of $h$ is decreased by a factor of $h$.

Piecewise-linear approximation. The approximating function $\tilde{f}(x)$ was represented in the form

$$\tilde{f}(x) = A_r + K_r (x - z_r), \quad z_r \leq x \leq z_{r+1}, r = 0, N_a - 1,$$

at what $z_0 = x_0, z_{N_a} = x_N, \tilde{f}(z_r) = f(z_r); \quad |\tilde{f}(x) - f(x)| \leq \varepsilon$ for $x \in [a, b]$.

Function $\tilde{f}(x)$ is defined by the table $(z_r, A_r, K_r)_{r=0}^{N_a}; z_r$ - nodes, $N_a$ - number of nodes, $H_r = z_{r+1} - z_r$ - approximation intervals, $K_r$ - angular coefficients, $z_0 = x_0, \quad A_0 = f_0, \quad A_{r+1} = A_r + K_r H_r$ (continuity $\tilde{f}(x)$).

Thus, the piecewise linear approximation is determined by the parameters $K_r, H_r, r \geq 0$. The maximum of $H_r$ is determined by the choice of point $z_{r+1}, r \geq 0$, as far removed from $z_r$;

$$|\tilde{f}(x) - f(x)| \leq \varepsilon, x \in [z_r, z_{r+1}], \tilde{f}(x) = f(x), \tilde{f}(z_{r+1}) = f(z_{r+1}).$$

Calculation $z_r, A_r, K_r$. Accepted $z_0 = x_0, A_0 = f_0$. The calculated values of $z_r, A_r$ are $z_{r+1}$, $H_r = z_{r+1} - z_r, A_{r+1} = f(z_{r+1}), K_r = \frac{A_{r+1} - A_r}{H_r}$ (point $z_{r+1}$ is one of the tabulation points $x_j$).

The algorithm for piecewise linear approximation of the kinetic process $f(x)$ with intervals of maximum length on segment $[a, b]$ is proposed below.

The calculation algorithm $z_{r+1}$ is reduced to the choice of the tabulation point $x_j > z_r$, taking into account condition

$$\max_{j_r, v \leq j_r} \left| A_r - f_j - A_j \right| \leq \varepsilon; \quad (1)$$

where $j_r -$ the number of the tabulation point $x_{j_r}$, which corresponds to $z_i (z_r = x_{j_i})$.

As soon as for some $j$ the condition (1) is violated, we store $z_j$ as $x_j$ (the number is remembered $K_r^0 = \frac{f_j - A_r}{x_j - z_r}, A_{r+1}^0 = f_j$ as $x_j$) and is accepted. Then condition (1) for $x_j > z_{r+1}$ is checked.
If \( \forall x_j \in \left[ z_{r+1}^0, x_N \right] \) condition (1) is not satisfied, is accepted \( z_{r+1} = z_{r+1}^0, A_{r+1} = A_{r+1}^0, K_r = K_r^0, j_{r+1} = j_{r+1}^0 \) and proceed to the calculation of \( z_{r+2} \).

If condition (1) is satisfied for some \( x_j \in \left[ z_{r+1}^0, x_N \right] \), then the transition to the previous stage is performed (\( r \) does not increase).

This will define all the triads \( \{z_., A_., K_r\}_{r=0}^{N-1} \). In the last triad \( \{z_{N_e}, A_{N_e}, K_{N_e}\} \), it suffices to compute \( z_{N_e} = z_{r+1} = x_N, K_r = K_{N_e-1} \).

Note that if \( f(x) \) satisfies condition \( \|f(x)\| \geq \alpha \forall x \in [a, b] \), then instead of condition (1) (using the averaged relative error \( \bar{\epsilon}_a = \frac{\|\tilde{f} - f\|}{f_{cp}} \times 100\% \)), one can also use condition

\[
\max_{j, i \in \mathbb{I}} \left| f_i - f_j - A_r \frac{x_j - z_r}{x_i - z_r} (x_i - z_r) \right| \leq \frac{\epsilon_0}{100} |f_i|.
\]

If, when condition (1) \( x_j = x_N \) is satisfied, then \( z_{N_e} = z_{r+1} = x_N, K_r = K_{N_e-1} = \frac{f_N - A_r}{x_N - z_r} \); the calculations are completed.

3. Approximation by cubic splines

We also give another possible version of the approximation of the kinetic process, based on the use of interpolation by polynomials in individual sections, and not on the basis of constructing a global interpolation polynomial over the whole interval. The smooth piecewise polynomial functions (composed of polynomials of the same degree) obtained in this case are splines. We confine ourselves to cubic splines (composed of polynomials of the third degree). We propose an algorithm for constructing cubic splines of class \( C^2 \) (twice continuously differentiable functions).

Here it is assumed that the values of the function \( f(x) : f_i = f(x_i), i = 1, N \). Are given in grid \([a, b]\) at grid nodes \( \text{ord}[a = x_1 < x_2 < \ldots < x_N = b] \). According to the preceding, the interpolating cubic spline \( S(x) \) must satisfy the following conditions:

\[
S(x_i) = f_i, \quad S'(x_i) = f'(x_i), \quad S''(x_i) = f''(x_i).
\] (2)

The cubic spline \( S(x) \) on each of the segments \([x_i, x_{i+1}]\) is determined by four coefficients; for its construction on the whole interval \([a, b]\) it is required to determine \( 4N \) coefficients. From the condition that the spline belongs to the class \( C^2 \), it is assumed that all internal interpolation points \( x_i, i = 1, N - 1 \), not only the spline \( S(x) \), but its derivatives \( S'(x) \) and \( S''(x) \) are continuous. From these conditions we obtain \( 3(N - 1) \) equations for determining the unknown spline coefficients. Adding \( N + 1 \) equation from (2), we have \( 4N - 2 \) equations; we obtain two missing equations from the boundary conditions (restrictions on the values of the spline and its derivatives at the ends of the interval). The following boundary conditions are most commonly used:

I. \( S'(a) = f'(a), S'(b) = f'(b) \)
II. \( S''(a) = f''(a), S''(b) = f''(b) \)
III. \( S^k(a) = S^k(b), k = 1, 2 \)
IV. \( S''(x_p + 0) = S''(x_p - 0), \quad p = 1, N - 1 \)

The so-called "natural" conditions have the form: \( S'(a) = 0, \quad S''(b) = 0 \).

At each of the intervals \([x_i, x_{i+1}]\) the spline is not represented in general form

\[
S(x) = a_i + b_i x + c_i x^2 + d_i x^3,
\]

but in some special, allowing to reduce the number of unknown spline coefficients. For this we introduce the notation: \( S'(x_i) = m_i, i = 0, N; \quad h_i = x_{i+1} - x_i, \quad t = \frac{x - x_i}{h_i}. \)

On segment \([x_i, x_{i+1}]\) the cubic spline can be written in the form

\[
S(x) = f_i (1 - t)^2 (1 + 2t) + f_{i+1} t^2 (3 - 2t) + m_i h_i (1 - t)^2 - m_{i+1} t^2 (1 + t) h_i.
\]

On each of the intervals \([x_i, x_{i+1}]\) it is continuous along with its first derivative everywhere on \([a, b]\). We choose parameters in such a way that the second derivative is also continuous at all internal nodes. We obtain the following system of equations:

\[
\lambda_i m_{i-1} + 2 m_i + \mu_i m_{i+1} = 3 \left( \mu_i \frac{f_{i+1} - f_i}{h_i} + \lambda_i \frac{f_i - f_{i-1}}{h_{i-1}} \right),
\]

Where \( \mu_i = \frac{h_i}{h_i - h_{i+1}}, \lambda_i = 1 - \mu_i = \frac{h_i}{h_i + h_{i+1}}, i = 0, N \).

Equations (3) should be supplemented by equations

\[
2m_0 + m_1 = 3 \frac{f_1 - f_0}{h_0}, \quad m_{N-1} + 2m_N = 3 \frac{f_N - f_{N-1}}{h_{N-1}},
\]

obtained from the boundary conditions.

The problem of constructing a cubic spline has been reduced to solving a linear system for the unknown coefficients \( m_i \):

\[
2m_0 + m_1 = 3 \frac{f_1 - f_0}{h_0}, \quad \lambda_i m_{i-1} + 2m_i + \mu_i m_{i+1} = 3 \left( \mu_i \frac{f_{i+1} - f_i}{h_i} + \lambda_i \frac{f_i - f_{i-1}}{h_{i-1}} \right),
\]

\[
m_{N-1} + 2m_N = 3 \frac{f_N - f_{N-1}}{h_{N-1}}.
\]

In solving practical problems, system (4) was solved taking into account tridiagonality of the matrix of the system.

4. Approximation by special functions

When solving a whole series of problems in the study of composite materials as nonstationary dynamical systems, it becomes necessary to approximate not only the input and output signals (the "black box"), but also the determination of particular transfer functions (the parameters of coupling the output signals to the input signals). We used for this the decomposition of the kinetic process over various orthonormal systems of special functions, the preference was given to Laguerre polynomials [5]:

\[
L_n(t) = \sum_{\nu=0}^{n} \frac{n!(-t)^\nu}{\nu! (n - \nu)!} ; \quad \int_0^\infty L_n(t) L_m(t) e^{-t} dt = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases},
\]

since in this case the transfer function \( W(p) \) is easily defined as a rational function \( \frac{Y(p)}{X(p)} \) with simple rules for calculating the coefficients.
In solving practical problems, the human factor also plays an important role: the choice of the form of the approximating function is often determined by the intuition of the experimenter. Thus, according to Table 1, we determined the analytical dependence of the viscosity $B$ of the epoxy composite on the temperature $t$, °C, and the percentage content $x$, % of a special additive.

| $x$ | 50 | 55 | 60 | 65 | 70 | 75 | 80 | 85 | 90 | 95 | 100 |
|-----|----|----|----|----|----|----|----|----|----|----|-----|
| 0   | 172| 119| 84 | 65 | 50 | 40 | 30 | 25 | 22 | 20 | 19  |
| 1   | 210| 145| 105| 80 | 65 | 52 | 43 | 35 | 30 | 27 | 25  |
| 5   | 250| 160| 115| 90 | 75 | 60 | 48 | 40 | 33 | 30 | 28  |
| 10  | 97 | 65 | 45 | 33 | 22 | 17 | 10 | 11 | 9  | 8  |     |
| 15  | 132| 91 | 62 | 47 | 36 | 30 | 21 | 18 | 17 | 15 | 12  |

Proceeding from the cognitive analysis [6,7], the approximating function was given in the form $B = B(t,x)$. Function $B = B(t,x) = \text{const}$ was represented as a polynomial of the third degree, and $B = B(\text{const},t)$ - functions of the form $y = a e^{-kt}$, $k = k(x)$ for different degrees of the polynomial. Based on these results, an approximation was obtained

$$B = \left(c_0 + c_1 x + c_2 x^2 + c_3 x^3\right) e^{r(x)(t-50)}, \quad 50 \leq t \leq 100.$$

5. Conclusion

The methods of approximation of the kinetic processes of the formation of physicomechanical characteristics are proposed for synthesis of composite materials with a regulated structure and properties:
- approximation of kinetic processes with the possibility of selecting the maximum length of partial intervals;
- algorithm of approximation by cubic splines;
- applications of Laguerre polynomials to the definition of interelement bonds in composite materials, as complex dynamic systems.

The proposed methods have been tested in the development of a number of special-purpose composite materials.

References
[1] Garkina I.: Modeling of kinetic processes in composite materials. Contemporary Engineering Sciences. 9(8) (2015) 421-425.
[2] Irina Garkina and Alexander Danilov: Mathematical Methods of System Analysis in Construction Materials. IOP Conf. Series: Materials Science and Engineering. 245 (2017) 062014.
[3] Irina Garkina, Alexander Danilov: Analytical design of building materials. Journal of Basic and Applied Research International. 18(2) (2016) 95-99.
[4] Garkina, A. Danilov, Y. Skachkov: Modeling of Building Materials as Complex Systems, Key Engineering Materials. 730 (2017) 412-417.
[5] G. Beytmen, A. Erdeyi: The highest transcendental functions. M.: Science. Vol. 2 (1973) 297 p.
[6] Garkina I., Danilov A.: Tasks of Building Materials from the Viewpoint of Control Theory, Key Engineering Materials. 737(2017) 578-582.
[7] Garkina I.A., Danilov A.M.: Experience of development of composite materials: some aspects of mathematical modeling. News of higher educational institutions. Construction. 8 (656) (2013) 28-33.