Modeling of deformation-strength characteristics of polymer concrete using fractional calculus

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Abstract. We consider a second-order differential equation containing a derivative of a fractional order (the Bagley-Torvik equation) in which the order of the derivative is in the range from 1 to 2 and is not known in advance. This model is used to describe oscillation processes in a viscoelastic medium. To study the equation, we use the Laplace transform, which allows us to obtain in an explicit form the image of the solution of the corresponding Cauchy problem. Numerical solutions are constructed for different values of the parameter. On the basis of the solution obtained, a numerical technique is proposed for parametric identification of an unknown order of a fractional derivative from the available experimental data. On the range of possible values of the parameter, the least-squares deviation function is determined. The minimum of this function determines the desired value of the parameter. The approbation of the developed technique on experimental data for polymer concrete samples was carried out, the fractional derivative parameter in the model was determined, the theoretical and experimental curves were compared, the accuracy of the parametric identification and the adequacy of the technique were established.

1. Introduction
Condensing polymers, due to their inherent complex of valuable properties, find the widest application in various fields of engineering. The advanced monomers and modifiers for the production of self-extinguishing and nonburning polymers are the condensation products of chloral (trichloroacetalddehyde) with aromatics. The production of chloral, an intermediate material for the synthesis of high-polymeric disinsectants, was established on a large scale in most industrialized countries. But because of the toxicity of high-polymeric disinsectants, they were withdrawn from production. And the task was to use the established production of chloral and its derivatives for other purposes [1].

Therefore, since 1962 [2] complex studies have been initiated to use chloral and its derivatives for the synthesis of polymers. It should be noted [3] that chloral derivatives have been used for a long time to produce nonburning polymeric esters with high strength characteristics.

The use of chloral derivatives for the production of polymer concrete with reduced flammability has only recently been launched and is a very urgent task. In connection therewith, new methods are
needed for calculating the strength properties of the corresponding polymer concretes (see the thesis [4] and the literature therein).

2. Bagley-Torvik equation and Laplace transform

Functionals of fractional differentiation find wide application in the description of oscillating processes. It is known [5–7] that equations containing fractional derivatives effectively describe moving structures containing elastic and elastic-plastic elements. These equations also describe damped motions with fractional damping, in particular, rock shakes of subsurface rocks [8], bounces of nanoscale sensors, etc. [9, 10], and also serve as a basis for considering nonlinear oscillating processes [11].

The problem is considered

\[ u'' + c D^\alpha u + \lambda u = 0 \]

\[ u(0) = 0, \quad u'(0) = 1, \]

where \( D^\alpha u \) is the fractional derivative of order \( \alpha \). When \( 1 < \alpha < 2 \), according to the definition of Riemann-Liouville, it is written in the form [12]

\[ D^\alpha u = \frac{d^2}{dx^2} \left[ \frac{1}{\Gamma(2 - \alpha)} \int_0^x u(t) dt \right] \]

For the first time, the equation (1) was proposed by Bagley and Torvik [13, 14] for modeling the damping properties of various elastic-plastic materials (polymers, glasses, etc.). These theses aroused much interest, which has not weakened so far [15].

In one of the recent theses [4], this scheme was used in modeling the change in the deformation-strength characteristics of polymer concrete when subjected to loadings. Samples of polymer concrete based on polyester resin (diane and diacyl chloride-1,1-dichloro-2,2-diethylene) were investigated. Polymer concrete is represented as a set of granules of mineral extender in an elastic-plastic medium. In this case, the motion of the granule \( u \) is described by the equation (1), where \( c \) – the viscosity modulus of the resin, \( \lambda \) – the rigidity modulus of the resin, \( \alpha \) – the elastic-plastic parameter of the medium.

It is noteworthy that the mechanical systems described by the equation (1) are very sensitive to changes in the order of fractional damping. In this connection, the most important problem of parametric identification of this value arises. With undiminishing interest in such oscillation systems, the question of parametric identification [16] remains insufficiently studied.

In this thesis, the solution of problem (1) is expressed through the Laplace integral and a technique is proposed for parametric identification of the order of the fractional derivative from experimental data.

We integrate the equation (1) from 0 to \( x \) and transform the expression.

\[ \int_0^x u''(t) dt + c \int_0^x D^\alpha u(t) dt + \lambda \int_0^x u(t) dt = 0, \]

\[ \int_0^x u'(t) dt + \frac{c}{\Gamma(2 - \alpha)} \int_0^x u(t) dt \frac{d^2}{dt^2} \left[ \int_0^\tau u(\tau) d\tau \right]^{x - \tau - 1} + \lambda \int_0^x u(t) dt = 0, \]

\[ u'(x) - u'(0) + \frac{c}{\Gamma(2 - \alpha)} \frac{d}{dt} \left[ \int_0^\tau u(\tau) d\tau \right]^{x - \tau - 1} + \lambda \int_0^x u(t) dt = 0, \]

\[ u'(x) - 1 + \frac{c}{\Gamma(2 - \alpha)} \frac{d}{dx} \left[ \int_0^x u(t) dt \right]^{x - x - 1} + \lambda \int_0^x u(t) dt = 0. \]
\[ \int_0^s u'(t) \, dt - \int_0^s dt + \frac{c}{\Gamma(2-\alpha)} \int_0^s d_\tau \left[ \frac{u(\tau) \, d\tau}{(t-\tau)^{\alpha-1}} \right] + \lambda \int_0^s u(\tau) \, d\tau = 0, \]

\[ u(x) - x + \frac{c}{\Gamma(2-\alpha)} \int_0^s (x-t)^{1-\alpha} u(t) \, dt + \lambda \int_0^s u(\tau) \, d\tau = 0. \tag{4} \]

For solving the equation (4), we use the Laplace transformation.
Let \( U(s) \) is the image of \( u(x) \), that is \( U(s) = u(t) \), or, which is the same \[17\]

\[ U(s) = \int_0^\alpha e^{-st} u(t) \, dt. \]

We assume that the solution of the equation (4) is in the class of functions for which the Laplace integral converges.

The function

\[ \int_0^\alpha (x-t)^{1-\alpha} u(t) \, dt \]

is a resultant of the functions \( u(x) \) and \( x^{1-\alpha} \). Indeed, by the definition, the resultant of two functions \( f_1(x) \) and \( f_2(x) \) is the function

\[ F(x) = \int_0^\alpha f_1(t) f_2(x-t) \, dt. \]

There is a simple images formula for resultant of functions

\[ \int_0^\alpha f_1(t) f_2(x-t) \, dt = F_1(s) F_2(s), \]

where \( F_1(s) \) and \( F_2(s) \) are the images of the functions \( f_1(x) \) and \( f_2(x) \) respectively.

As is known, the image of the power function \( x^\mu \) when \( \mu > -1 \) is equal to \( \Gamma(\mu+1)s^{-\mu} \). Thus

\[ \int_0^\alpha (x-t)^{1-\alpha} u(t) \, dt = U(s) s^{\alpha-2} \Gamma(2-\alpha). \tag{5} \]

It's obvious that

\[ \int_0^\alpha u(\tau) \, d\tau = \int_0^\alpha u(\tau) \, d\tau = \frac{U(s)}{s^\alpha}. \tag{6} \]

Thus, applying the Laplace transformation to (4) and taking into account relationships (5) and (6), we obtain the equation for the image of the solution

\[ U(s) - \frac{1}{s^\alpha} + cU(s)s^{\alpha-2} + \lambda \frac{U(s)}{s^\alpha} = 0. \]

From this we obtain the formula for the image

\[ U(s) = \frac{1}{s^\alpha + cs^{\alpha-2} + \lambda}. \tag{7} \]

The formula (7) allows us to express the solution of problem (1) through the Laplace integral

\[ u(x) = \frac{1}{2\alpha} \int_{e^{-ic}}^{e^{ic}} e^{\alpha s} U(s) \, ds. \tag{8} \]
2.1. Numerical solutions

Graphs of solutions according to formula (8) can be set up numerically [18]. The calculations were carried out in Mathcad 14. The Fig. 1 shows graphs for different values of $\alpha$. The remaining parameters are taken as follows $c = 1.8, \lambda = 93$. These parameter values were obtained during experiments on samples of polymer concrete [4].

![Graphs of solutions when $1 < \alpha < 2$.](image)

Numerical verification confirms the correctness of the limit behavior of the solution, which transforms into harmonic oscillations at values of $\alpha$ close to 2.

3. Experimental data and parameter identification

The possibility of calculating the solution at any point makes it possible to develop a simple and effective technique for parametric identification of a parameter of $\alpha$ from experimental data, assuming that the remaining parameters of the equation are known (with some degree of accuracy). In contrast to the spectral method [16], this technique is quite simple in practical implementation.

Let us assume that several experimental points are known, they are $u(x_i) = U_i$, $i = 1, ..., N$. The unknown parameter $\alpha$ can be selected by minimizing the deviation of the theoretical curves from the experimental ones. Theoretical points can be calculated by the formula (4) $u(x, \alpha)$. We define the function of deviation by the least square method

$$F(\alpha) = \sum_{i=1}^{N} (U_i - u(x_i, \alpha))^2$$

(9)

This function represents the sum of the deviations of the theoretical points from the experimental points. The value $\alpha$, that minimizes this function can be approximately considered the desired one. The accuracy of identification depends on the number of experimental points, as well as the accuracy of other system parameters.

The advantage of this technique of parametric identification in comparison with various nomographic methods [19, 20] consists in the exact quantitative evaluation of the choice of the desired parameter. In addition, the deviation function (9) can be set up over the entire range of the assumed parameter values, which increases the accuracy of the identification.

In the experimental studies [4], samples of polymer concrete based on polyester resin (diane and diacyl chloride-1,1-dichloro-2,2-diethylene) were placed in the isothermal chamber in the test facility (Figure 2) in order to exclude the effect of temperature on the experimental results. Studies were carried out on samples of 0.57 mm × 480 mm at a constant temperature of 25 °C. The data obtained as a result of a series of tests are presented in Table 1.
Figure 2. Test Facility in the Isothermal Chamber

Table 1. Experimental Relationship between Time and Deformation for Polymer Concrete Samples

| Time (s) | Deformation (relative) |
|---------|------------------------|
| 0.25    | 0.05                   |
| 0.5     | -0.04                  |
| 0.75    | -0.01                  |
| 1       | 0.02                   |
| 1.25    | -0.01                  |
| 1.5     | -0.01                  |

According to these data, we set up the deviation function (9). The Fig. 3 shows the graph of the deviation function.
From the graph it follows that the deviation function has the minimum at \( \alpha \approx 1.47 \). It can be assumed that the order of the fractional derivative in (1) is equal to this value. Of course, there is some error associated with the measurement error and the determination of other parameters. The Fig. 4 shows the experimental points and the theoretical curve.

Comparison of the experimental data with the model allows to draw a conclusion about the adequacy of modeling and high accuracy of the parametric identification technique. The stability of model solutions to small oscillations of the order of the fractional derivative was also established earlier that confirms the correctness of the obtained values. Knowledge of the model parameter allows, for example, to predict the deformation-strength characteristics of the material (polymer concrete, asphalt concrete, etc.) when subjected to loadings.
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