The fractional derivative type identification for the modelling deformation and strength characteristics of polymer concrete

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Abstract. The article contains the comparative use analysis of fractional derivative three types (Riemann-Liouville, Caputo and model) at the Begley-Torvik equation when modeling the deformation and strength characteristics of polymer concrete. We also consider how to obtain a solution to the Begley-Torvik equation initial value problem for the fractional derivative model using a recurrent kernels sequence. Further, the correctness is substantiated of establishing the type and the fractional derivative order at the Begley-Torvik equation initial value problem.

1. Introduction
Differential equations containing a fractional derivative are currently actively used to construct mathematical models at various fields of natural science. The work [1] is a unique comprehensive review on the fractional calculus theory and its application. It should be noted that both the study of solutions to equations and inverse problems are relevant - determining which kind of equation is the best mathematical model of the studied physical or other process.

Consider an initial value problem of the form:

\[ u''(x) + cD^\alpha u(x) + \lambda u(x) = 0; \quad x \in [0; \infty); \]
\[ u(0) = 0; \quad u'(0) = c \neq 0; \]  

where \( D^\alpha u(x) \) is the fractional differentiation operator.

Depending on the process under study, the operator \( D^\alpha \) can be the fractional differentiation operator by the Caputo definition of order \( \alpha \), \( 1 < \alpha \leq 2 \):

\[ D^\alpha u(x) = \frac{1}{\Gamma(2-\alpha)} \int_0^x \frac{u''(\tau)d\tau}{(x-\tau)^{\alpha-1}}, \]  

where \( \Gamma \) - gamma function; or the operator \( D^\alpha \) can be the fractional differentiation operator by the Riemann-Liouville definition, where \( 1 < \alpha \leq 2 \):

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

or the operator \( D^\alpha \) can be a fractional differentiation model operator [2], where \( 1 < \alpha \leq 2 \)

\[ D^\alpha u(x) = \frac{d}{dx} \left( \frac{1}{\Gamma(2-\alpha)} \int_0^x \frac{u'(\tau)d\tau}{(x-\tau)^{\alpha-1}} \right). \]
The results of solving problem (1) - (2) are used to simulate changes in the deformation and strength characteristics of polymer concrete when subjected to loadings. Polymer concrete is the mineral filler granules set in a viscoelastic medium. In this case, the constants included at the equation have the following physical meaning: \( \varepsilon \) is the viscosity modulus of resin, \( \lambda \) is the rigidity modulus of resin, \( \alpha \) is the parameter of viscoelasticity of resin. From [3] it is known that for polymer concrete based on polyester resin (diane and dichloroanhydride - 1,1 - dichloro - 2,2 - diethylene), the values of the parameters of equation (1) are \( \varepsilon = 1.8; \lambda = 93 \).

2. Methods

The problem solution (1) - (2) can be found by the recurrent kernels sequence [4] and written at the form of a power series for the Riemann-Liouville fractional differentiation operator:

\[
u_{RL}(x) = c \left( x + \sum_{n=1}^{\infty} (-1)^n \sum_{m=0}^{n} \frac{n!}{m!(n-m)!} \frac{\lambda^n m^n}{\Gamma(2n+2m\alpha)} x^{2n+1-\alpha} \right)
\]

or for the Caputo fractional differentiation operator

\[
u_{C}(x) = c \left( x - \frac{\lambda x^3}{6} + \sum_{n=1}^{\infty} (-1)^n \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} \frac{\lambda^n}{\Gamma(n+1-k\alpha)} x^{2n+3-k\alpha} \right).
\]

Consider the initial value problem solution (1) - (2) for the model fractional derivative (5) using the recurrent kernels sequence. For this, we introduce into consideration the function

\[z(x) = u'(x).\]

Then using (2):

\[u(x) = \int_0^x u'(\tau)d\tau + u(0) = \int_0^x z(\tau)d\tau\]

We obtain from (1) - (2) the initial value problem for the function \( z(x) \):

\[z'(x) + \frac{\varepsilon}{\Gamma(z-\alpha)} \int_0^x \frac{z(\tau)d\tau}{(x-\tau)^{\alpha}} + \lambda \int_0^x z(\tau)d\tau = 0; \quad x \in [0; \infty]; \quad z(0) = c.
\]

We have from (8) by integration:

\[z(\xi) - z(0) + \frac{\varepsilon}{\Gamma(z-\alpha)} \int_0^\xi \frac{z(\tau)d\tau}{(\xi-\tau)^{\alpha}} + \int_0^\xi \lambda(\xi - x)z(x)d\tau = \tilde{c}; \quad \xi \in [0; \infty].
\]

In the last equation, we change the order of integration, then

\[z(\xi) - z(0) + \frac{\varepsilon}{\Gamma(z-\alpha)} \int_0^\xi \frac{z(\tau)d\tau}{(\xi-\tau)^{\alpha}} + \int_0^\xi \lambda(\xi - x)z(x)d\tau = \tilde{c}; \quad \xi \in [0; \infty].
\]

Setting \( \xi = 0 \), we obtain that \( \tilde{c} = 0 \). We arrive, using (9), to the Volterra integral equation of the second kind (which we write using the variable \( x \)):

\[z(x) + \int_0^x \left\{ \frac{\varepsilon}{\Gamma(z-\alpha)} (x - \zeta)^{-\alpha} + \lambda(x - \zeta) \right\} z(\zeta)d\zeta = c; \quad x \in [0; \infty].
\]

The equation solution (10) is

\[z(x) = z_0(x) - z_1(x) + \cdots + (-1)^n z_n(x) + \cdots,
\]

where

\[z_0(x) = c;
\]

\[z_n(x) = \int_0^x \left\{ \frac{\varepsilon}{\Gamma(z-\alpha)} (x - \zeta)^{-\alpha} + \lambda(x - \zeta) \right\} z_{n-1}(x)d\zeta , n = 1; 2; \ldots
\]
We find the integrals, applying the mathematical induction method:

\[ z_n(x) = c \sum_{k=0}^{n} \frac{n!}{k!} \lambda^{n-k} \frac{x^{2n-k}}{\Gamma(2n+1-k\alpha)} \]

Then

\[ z(x) = c \left\{ 1 + \sum_{n=1}^{\infty} (-1)^n \sum_{k=0}^{n} \frac{n!}{k!} \lambda^{n-k} \frac{x^{2n-k}}{\Gamma(2n+1-k\alpha)} \right\} \]

We have:

\[ u(x) = c \left\{ x + \sum_{n=1}^{\infty} (-1)^n \sum_{k=0}^{n} \frac{n!}{k!} \lambda^{n-k} \frac{x^{2n+1-k\alpha}}{\Gamma(2n+2-k\alpha)} \right\} \]

Thus, under conditions (2), the equation solution (1) with the model fractional derivative coincides with the equation solution (1) with the Riemann-Liouville fractional derivative.

Problem (1) - (2) consists in finding a solution \( u(x) \); \( x \in [0; \mathbb{R}] \) satisfying equation (1) with known parameters \( c, \lambda, \alpha \) and conditions (2) with a known constant value \( c \). The inverse problem can be formulated as follows: if the equation solution (1) with parameters \( \lambda \) and \( \varepsilon \) is known, then the function \( u(x) ; x \in [0; \mathbb{R}] \) for which conditions (2) are satisfied, then what is the order value of the fractional derivative \( \alpha \) and the constant \( c \)?

In [5], it was obtained by the least squares method that if we take the value \( c = 1 \) in (2) and use the fractional derivative according to Riemann-Liouville, then its order is \( \alpha = 1.47 \). The application of the least squares method is caused by the existence of an error during the experiment and the processing of its results.

3. Results

e will determine which type of fractional derivative best describes the processes in polymer concrete under the action of loads. As initial data, we will use the values \( \{(x_j; U_j)\}_{j=1;2;...;6} \) for polymer concrete samples based on polyester resin (diane and dichloroanhydride - 1.1 - dichloro - 2.2 - diethylene) from work [5], which are presented in table.1.

| \( x_j \) | \( U_j \) |
|---|---|
| 0.25 | 0.05 |
| 0.5 | -0.04 |
| 0.75 | -0.01 |
| 1 | 0.02 |
| 1.25 | -0.01 |
| 1.5 | -0.01 |

For \( \alpha \in [1.01; 1.65] \) with the 0.001 step by the variable \( \alpha \), for \( x \in [0.01; 1.51] \) with the 0.01 step by the variable \( x \); for \( c \in [0.5; 1.5] \) with the 0.01 step by the variable \( c \), we calculate the functions values by the form:

\[ u_{RL}(x, \alpha, c) = c \left\{ x + \sum_{n=1}^{100} (-1)^n \sum_{m=0}^{n} \frac{n!}{m!} (1.8)^{m} \alpha^{n-m} \frac{x^{2n+1-m\alpha}}{\Gamma(2n+2-m\alpha)} \right\} \] (11)
\[ u_c(x, \alpha, c) = c \left( x - \frac{93x^3}{6} + \sum_{n=1}^{100} (-1)^{n+1} \sum_{k=0}^{n} \frac{(n \choose k)k3^{n+1-k}x^{2n+3-ko}}{(2n+4-ko)} \right) \]  

(12)

Now we will compose the functions that characterize the deviations of the experimental data points \((x_j; U_j)\) from the points of the graphs of solutions to problem (1) - (2), calculated by formulas (11) and (12):

\[ H_{RL}(\alpha, c) = \sum_{j=1}^{6} (u_{RL}(x_j, \alpha, c) - U_j)^2 \]

\[ H_C(\alpha, c) = \sum_{j=1}^{6} (u_C(x_j, \alpha, c) - U_j)^2 \]

The minimum of the function \(H_{RL}(\alpha, c)\) is attained when \(\alpha = 1.472, c = 0.912\) and is

\[ H_{RL}(1.472, 0.91) = 5 \cdot 10^{-5} \]

and the minimum of the function \(H_C(\alpha, c)\) is attained when \(\alpha = 1.422, c = 0.495\) and is

\[ H_C(1.486, 0.92) = 10^{-3} \]

Accordingly the values of the parameters of initial value problem of the form (1) - (2) for polymer concrete based on polyester resin (diane and dichloroanhydride - 1,1 - dichloro - 2,2 - diethylene) are

\( \varepsilon = 1.8; \lambda = 93; \alpha = 1.472, c = 0.912. \)

Figure 1 shows the solutions graphs to problem (1) - (2) corresponding to those values of the fractional derivative order and the solution derivative at zero, at which the minimum of \(H_{RL}\) and \(H_C\) is reached, as well as data obtained as the experiment result.

![Graphs of the functions](image)

**Figure 1.** Graphs of the functions \(u_{RL}(x, 1.472, 0.912)\) and \(u_C(x, 1.422, 0.495)\) and experimental data.

The calculations show that the fractional derivative use the according to Riemann - Liouville is preferable when modeling the change in the deformation and strength characteristics of polymer concrete based on polyester resin (diane and dichloroanhydride - 1,1 - dichloro - 2,2 - diethylene) when subjected to loadings.

To confirm the statement correctness of the parametric identification problem with respect to the fractional derivative order, we numerically check the solution stability to a parameter \(\alpha\) variation. To do this, at the vicinity of the point \(\alpha\), consider the relative increment of this parameter by \(\Delta\alpha\) and define the deviation function at the \(L_2\) metric:
\[ \rho(\alpha; \delta) = \int_0^{\delta} (u(x, \alpha) - u(x, \alpha + \alpha \cdot \delta))^2 \, dx. \]

In this case, the partial derivative \( \varepsilon(\alpha; \delta) = \frac{\partial \rho}{\partial \delta} \) of the introduced function will determine the sensitivity of the solution to a change by \( \alpha \). Figures 2 and 3 shows the sections of the graphs of the functions \( \varepsilon(\alpha; \delta) \) at values of the fractional derivative \( \alpha = 1.35; \alpha = 1.4; \alpha = 1.45; \alpha = 1.5 \) for fractional derivatives according to Riemann - Liouville (left) and Caputo (right). This figure demonstrates that the sensitivity \( \varepsilon(\alpha; \delta) \) increases linearly with increasing \( \delta \), and with the order increase of the fractional derivative \( \alpha \), the growth rate increases. The growth rate \( \varepsilon(\alpha; \delta) \) is higher for the Caputo fractional derivative.

**Figure 2.** Sections of the graphs of functions \( \varepsilon(\alpha; \delta) \) for Riemann - Liouville fractional derivatives for \( \alpha = 1.35; \alpha = 1.4; \alpha = 1.45; \alpha = 1.5 \).

**Figure 3.** Sections of the graphs of functions \( \varepsilon(\alpha; \delta) \) for Caputo fractional derivatives for \( \alpha = 1.35; \alpha = 1.4; \alpha = 1.45; \alpha = 1.5 \).

Table 2 contains the coefficients \( k \) (with an accuracy of 3 decimal places) of a linear function approximating the sensitivity \( \varepsilon(\alpha; \delta) \) at 4 values of \( \alpha \):

\[ \varepsilon(\delta) = k \cdot \delta \]

The determination coefficient \( R^2 \) is from 0.992 to 0.996.

**Table 2.** Coefficients \( k \) of linear approximation of sensitivity \( \varepsilon(\alpha; \delta) \).

| Fractional derivative according to Riemann - Liouville | Fractional derivative according to Caputo |
|--------------------------------------------------------|--------------------------------------------|
| \( \alpha = 1.1 \)                                   | 0.012                                      | 0.019                                      |
| \( \alpha = 1.3 \)                                   | 0.014                                      | 0.028                                      |
| \( \alpha = 1.4 \)                                   | 0.015                                      | 0.038                                      |
| \( \alpha = 1.5 \)                                   | 0.019                                      | 0.058                                      |
4. Conclusions

Thus:

- under conditions (2), the equation solution (1) with the model fractional derivative coincides with the equation solution (1) with the Riemann - Liouville fractional derivative;
- the calculations show that the fractional derivative use the according to Riemann - Liouville is preferable when modeling the change in the deformation and strength characteristics of polymer concrete based on polyester resin (dian and dichloroanhydride - 1,1 - dichlor - 2,2 - diethylene) when subjected to loadings;
- for polymer concrete based on polyester resin (diane and dichloroanhydride - 1,1 - dichloro - 2,2 - diethylene), the values of the parameters of initial value problem of the form (1) - (2) are $\varepsilon = 1.8; \lambda = 93; \alpha = 1.472; c = 0.912$;
- the correctness of establishing the type and order of the fractional derivative in problem (1) - (2) has been substantiated.

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References

[1] Handbook of Fractional Calculus with Applications. 2019 1 – 8 ed Tenreiro Machado J A (Berlin/Boston, De Gruyter GmbH)
[2] Aleroev T, Aleroeva H 2019 Fractional Differential Equations. ed Kochubei A, Luchko Y (Berlin, Boston: De Gruyter) pp 21–46.
[3] Kekharsaeva E R, Pirozhkov V G 2016 Sbornik trudov 6-i vserossiiskoi nauchnoi konferentsii s mezhdunarodnym uchastiem im. I.F. Obraztsova i Iu.G. Ianovskogo ”Mekhanika kompozitsionnykh materialov i konstruktsii, slozhnykh i geterogennykh sred” (Moskow IPRIM RAN) pp 104–9
[4] Erokhin S V, Aleroev T S, Frishter L Iu 2015 International Journal for Computational Civil and Structural Engineering 11 issue 3 pp 77-81
[5] Aleroev T S, Erokhin S V 2019 Math Models Comput Simul 11 p 219