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MATHEMATICAL MODELLING OF NONLINEAR DYNAMICS IN ACTIVATOR-INHIBITOR SYSTEMS WITH SUPERDIFFUSION

The nonlinear dynamics in generalized activator-inhibitor systems with space fractional derivatives is studied. As an example, the Brusselator model and the reaction–diffusion model with cubic nonlinearity, in which the classical spatial differential operators are replaced by their fractional analogues, are considered. The fractional operator reflects the nonlocal behavior of superdiffusion. The spatially homogeneous, time independent solution has been found for each system. We have also studied its linear stability and determined instability conditions of both Hopf and Turing. It was established that the anomalous diffusion (superdiffusion) leads to the qualitative change of nonlinear dynamics in mentioned systems.

Keywords – reaction-diffusion system, fractional operator, superdiffusion, Brusselator model, cubic nonlinearity, Hopf and Turing instabilities, dissipative structures.

Introduction

Experimental observations of spiral waves, spatial dissipative structures with complicated symmetries in many physical, chemical and biological media have made reaction-diffusion systems the subject of numerous investigations. At the same time investigations have shown that diffusion in many real systems has anomalous character and cannot be described in terms of normal (Fickian) diffusion. These processes can be described using models with subdiffusion or superdiffusion. Unlike normal diffusion, which is characterized by the dependence of the mean square displacement of a randomly walking particle on time $\left\langle (\Delta r)^2 \right\rangle \sim t$, anomalous diffusion is characterized by the more general dependence

$$\left\langle (\Delta r)^2 \right\rangle \sim 2dK_\gamma t^\gamma ,$$

where d is the spatial dimension, K_γ is a generalized diffusion constant. For normal diffusion the exponent γ is equal 1 and constant $K_1 = D$ being the ordinary diffusion coefficient. For $\gamma < 1$, the diffusion process is slower than normal diffusion and is called subdiffusion. The randomly walking particle can wait a long time to make a finite jump. While for $\gamma > 1$, the diffusion is called superdiffusion and is characterized by higher diffusion rate, and so the particle will pass this distance faster than in the case of normal diffusion.

Subdiffusion often occurs in gels [1-3], in porous media [4-6], and polymers [7, 8], while superdiffusion has been observed in transport in nonhomogeneous rocks [9, 10], in turbulent flows [11, 12], and also in optics [13], in single-molecule spectroscopy [14].

Because of anomalous diffusion the mentioned processes can be adequately described only using fractional differential equations apparatus [15-18].

The effect of anomalous diffusion on dissipative structures formation in time fractional reaction-diffusion systems is studied, in particular, in [19-21].

In work [22] the linear stability analysis in the Brusselator model with superdiffusion showed that, unlike the case of normal diffusion, the Turing instability can occur even when diffusion of the inhibitor is slower than that of the initiator. Therefore, studying the models with superdiffusion is an essential and important problem.

In this work, we investigate generalized reaction-diffusion models with superdiffusion, namely the Brusselator model and the model with cubic nonlinearity. These mathematical models that we consider are the standard models with the only exception that the classical Laplacians are replaced by the fractional operators that reflect nonlocal behavior of superdiffusion.

Brusselator model with superdiffusion. Linear stability analysis

We consider the well-known reaction-diffusion model Brusselator [23], in which the classical spatial differential operators are replaced by their fractional analogues

$$\frac{\partial u(x,t)}{\partial t} = D_1 \Delta^{\alpha} u(x,t) + A - (B+1)u + u^2 v ,$$

$$\frac{\partial v(x,t)}{\partial t} = D_2 \Delta^{\alpha} v(x,t) + Bu - u^2 v . \tag{1}$$

The system (1) must be completed by the following conditions on the boundaries:

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=L} = \left.\frac{\partial v}{\partial x}\right|_{x=0} = \left.\frac{\partial v}{\partial x}\right|_{x=L} = 0 , \tag{2}$$

or periodic boundary conditions

$$u|_{x=0} = u|_{x=L} , \quad v|_{x=0} = v|_{x=L} ,$$

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=L} , \quad \left.\frac{\partial v}{\partial x}\right|_{x=0} = \left.\frac{\partial v}{\partial x}\right|_{x=L} , \tag{3}$$

where $u = u(x,t)$ is an activator variable and $v = v(x,t)$ is inhibitor one; D_1, D_2 are diffusion coefficients; A, B are external bifurcation parameters; $x \in [0, L]$ is a space coordinate; t is a time; α is the exponent of fractional operator. Besides, $1 < \alpha < 2$, in other words the system of equation (1) describes the case when the diffusion exhibits anomalous character, namely the diffusion process passes faster than the normal diffusion.

We consider the fractional derivative in the form [16-18]

$$\frac{\partial^{\alpha} f(x,t)}{\partial x^{\alpha}} = -\frac{1}{2\cos(\pi\alpha/2)}\left[\mathrm{D}_{+}^{\alpha} f(x,t) + \mathrm{D}_{-}^{\alpha} f(x,t)\right],$$

where for $1 < \alpha < 2$

$$\mathrm{D}_{+}^{\alpha} f(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_{-\infty}^{x} \frac{f(\xi,t)}{(x-\xi)^{\alpha-1}} d\xi , \quad \mathrm{D}_{-}^{\alpha} f(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_{x}^{\infty} \frac{f(\xi,t)}{(\xi-x)^{\alpha-1}} d\xi ,$$

or in a form defined by its action in Fourier space $F[\frac{\partial^{\alpha} f}{\partial x^{\alpha}}](k) = -k^{\alpha} F[f](k)$.

Then the fractional Laplacian Δ^{α} are replaced by such operator [15]

$$\Delta^{\alpha} \equiv -(-\Delta)^{\alpha/2} \quad (1 < \alpha < 2) ,$$

or, using Fourier transform

$$\mathrm{F}[\Delta^{\alpha} f](\mathbf{k}) = -\mathbf{k}^{\alpha}\, \mathrm{F}[f](\mathbf{k}) ,$$

where $(-\Delta)^{\alpha/2}$ is Riesz derivative [15] and $\Gamma(2-\alpha)$ is the Gamma function.

It should be noted that in the case $\alpha = 2$, we'll obtain the standard Brusselator model [23].

The spatially homogeneous and stationary solution of the system (1) with the boundary conditions (2) or (3) is obtained as solution of the system of algebraic equations

$$A-(B+1)u+u^2v=0\,,$$

$$Bu-u^2v=0\,.$$

So the critical point of the system (1) corresponding to a homogeneous stationary solution, is

$$u_s=A\,,\quad v_s=\frac{B}{A}\,.$$

If we consider the deviation of the solution from the critical point

$$U=u-A\,,\quad V=v-\frac{B}{A}\,,$$

then as a result, we obtain

$$\frac{\partial U}{\partial t}=D_1\Delta^{\alpha}U+(B-1)U+U^2V+\frac{B}{A}U^2+2AUV+A^2V\,,$$

$$\frac{\partial V}{\partial t}=D_2\Delta^{\alpha}V-BU-U^2V-\frac{B}{A}U^2-2AUV-A^2V\,. \tag{4}$$

The critical point is now given by $U=V=0$. Stability of homogeneous stationary solution of the system can be analyzed by linearization of the system nearby this solution. So we decompose the nonlinear functions in the right sides of system (4) into Taylor series nearby the critical point $U=V=0$.

Then the system can be transformed to a linear system which has the form

$$\frac{\partial \mathbf{u}(x,t)}{\partial t}=\widehat{F}(u)\mathbf{u}(x,t)\,, \tag{5}$$

where $\mathbf{u}(x,t)=\begin{pmatrix}U(x,t)\\ V(x,t)\end{pmatrix}$, $\quad \widehat{F}(u)=\begin{pmatrix}D_1\Delta^{\alpha}+B-1 & A^2\\ -B & D_2\Delta^{\alpha}-A^2\end{pmatrix}$.

Here, $\widehat{F}(u)$ is Frechet derivative.

If we substitute the solution in such a form

$$\mathbf{u}(x,t)=\begin{pmatrix}U(x,t)\\ V(x,t)\end{pmatrix}=\begin{pmatrix}U_0\\ V_0\end{pmatrix}\mathrm{e}^{\lambda t+ikx} \tag{6}$$

into the linear system (5), then we obtain the characteristic equation for determine eigenvalues λ

$$\det|F-\lambda I|=0\,,$$

where $F=\begin{pmatrix}-D_1k^{\alpha}+B-1 & A^2\\ -B & -D_2k^{\alpha}-A^2\end{pmatrix}$ is a matrix determined by the operator $\widehat{F}$,

or explicitly

$$\lambda^2-\left[B-1-A^2-(D_1+D_2)k^{\alpha}\right]\lambda+A^2+\left[D_1A^2-D_2(B-1)\right]k^{\alpha}+D_1D_2k^{2\alpha}=0\,.$$

Here k is a wave number.

The eigenvalues are

$$\lambda_{1,2}=\frac{trF\pm\sqrt{tr^2F-4\det F}}{2}\,,$$

where $trF=B-1-A^2-(D_1+D_2)k^{\alpha}$ is a trace of matrix F;

$\det F=A^2+\left[D_1A^2-D_2(B-1)\right]k^{\alpha}+D_1D_2k^{2\alpha}$ is its determinant.

If $trF=0$ on condition that $\det F>0$, we obtain the critical value of the parameter B_{cr}

$$B_{cr} = 1 + A^2 + (D_1 + D_2) k^{\alpha}. \quad (7)$$

New solutions that can exist above the curve of neutral stability will be oscillating with natural frequency determined by imaginary part of eigenvalue. However, these solutions will be characterized by trivial space dependence since in this case the first unsteady mode will be excited when $k = 0$. This is the conditions of Hopf bifurcation.

It will be a different situation if the characteristic equation will have real roots. In this case the condition of neutral stability will have the simply form $\lambda = 0$. Thus, we have

$$\det F = A^2 + \left[D_1 A^2 - D_2 (B - 1) \right] k^{\alpha} + D_1 D_2 k^{2\alpha} = 0 .$$

As a result, neutral stability curve can be written in the form

$$B = \frac{1}{k^{\alpha}} \left(1 + D_1 k^{\alpha} \right) \left(\frac{A^2}{D_2} + k^{\alpha} \right). \quad (8)$$

This is the condition of Turing stability boundary. In this case, one can observe the mechanism of the genesis of own wave length in the system, i.e. there is a spatial symmetry breakdown.

The reaction–diffusion model with cubic nonlinearity

We investigate the effect of anomalous diffusion on pattern formation also in the reaction-diffusion model with cubic nonlinearity

$$\frac{\partial u(x,t)}{\partial t} = D_1 \Delta^{\alpha} u(x,t) + u - \frac{1}{3} u^3 - v,$$

$$\frac{\partial v(x,t)}{\partial t} = D_2 \Delta^{\alpha} v(x,t) + u - v + A. \quad (9)$$

Under the boundary conditions (2) or (3) the spatially homogeneous and stationary solution exists in the system (9) which has such a form

$$u_s = \sqrt[3]{-3A}, \quad v_s = \sqrt[3]{-3A} + A.$$

We rewrite the system of equations (9) in terms of the deviation of the solution from the critical point by introducing

$$U = u - \sqrt[3]{-3A}, \quad V = v - \sqrt[3]{-3A} - A.$$

Thus, we get

$$\frac{\partial U}{\partial t} = D_1 \Delta^{\alpha} U + (1 - \sqrt[3]{9A^2}) U - V + \sqrt[3]{3A} U^2 - \frac{1}{3} U^3,$$

$$\frac{\partial V}{\partial t} = D_2 \Delta^{\alpha} V + U - V. \quad (10)$$

We carry out linearization of the system (10) nearby the homogeneous stationary solution $U = V = 0$. As a result, we obtain

$$\frac{\partial \mathbf{u}(x,t)}{\partial t} = \hat{F}(u) \mathbf{u}(x,t), \quad (11)$$

where $\mathbf{u}(x,t) = \begin{pmatrix} U(x,t) \\ V(x,t) \end{pmatrix}$, $\quad \hat{F}(u) = \begin{pmatrix} D_1 \Delta^{\alpha} + 1 - \sqrt[3]{9A^2} & -1 \\ 1 & D_2 \Delta^{\alpha} - 1 \end{pmatrix}$.

The dispersion relation is

$$\lambda^2 + M_1 \lambda + M_2 = 0,$$

$$M_1 = \sqrt[3]{9A^2} + (D_1 + D_2)k^{\alpha},$$

$$M_2 = \sqrt[3]{9A^2} + \left[D_1 - \left(1 - \sqrt[3]{9A^2}\right)D_2\right]k^{\alpha} + D_1 D_2 k^{2\alpha}.$$

We are particularly interested in the Turing stability boundary, which corresponds to $\lambda = 0$. Then the neutral stability curve can be written in the form

$$A = \frac{1}{3}\sqrt{\left(\frac{D_2 k^{\alpha} - D_1 k^{\alpha} - D_1 D_2 k^{2\alpha}}{1 + D_2 k^{\alpha}}\right)^3}. \tag{12}$$

The curve has a single minimum (A_{cr}, k_{cr}):

$$A_{cr} = \frac{1}{3}\left[1 + \frac{D_1}{D_2} - 2\sqrt{\frac{D_1}{D_2}}\right]^{3/2}, \quad k_{cr} = \frac{1}{3}\left[\frac{1}{\sqrt{D_1 D_2}} - \frac{1}{D_2}\right]^{1/\alpha}.$$

In conclusion, we obtain the Turing instability threshold A_{cr} and also the critical value of the wave number k_{cr}, which depends on exponent α.

Numerical simulations

Systems of equations (1), (9) have been reduced to the corresponding systems of ordinary differential equations. For that we considered an analytical grid with nodes at the points $x_i = (i-1)h,\ h = L/(N-1),\ i = \overline{1,N}$. Fractional derivatives were approximated using schemes based on Grünwald-Letnikov and Riemann-Liouville definitions for $1 < \alpha < 2$ [24].

As a result for Riesz fractional derivative we have obtained such formula:

$$\Delta^{\alpha} U_i \approx -\frac{1}{2\cos\left(\frac{\pi\alpha}{2}\right)}\left(\sum_{k=0}^{i+1} c_k U_{i-k+1} + \sum_{k=0}^{i+1} c_k U_{i+k-1}\right),$$

where $c_0 = \dfrac{1}{h^{\alpha}},\quad c_k = c_{k-1}\cdot\left(1 - \dfrac{1+\alpha}{k}\right),\quad k = 1, 2, 3, \ldots$.

The results of numerical simulations are shown below.

Figure 1 presents characteristic view of dissipative structures for the system (1) for $A = 1$, $B = 3,\quad D_1 = 0.04,\quad D_2 = 1,\quad \alpha = 2$, i.e. for derivative of integer order $\alpha = 2$. In figure 2 we can see characteristic view of dissipative structures for fractional derivative, namely for $\alpha = 1.5$.

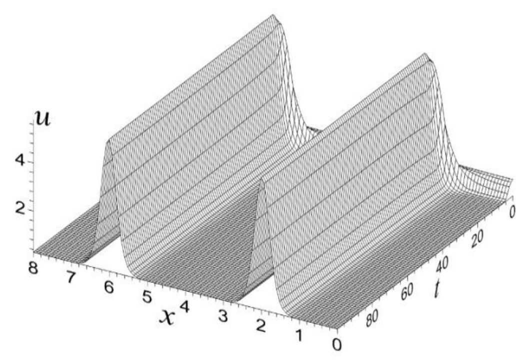

Fig. 1. Dynamics of variable u for $\alpha = 2$ (the Brusselator model)

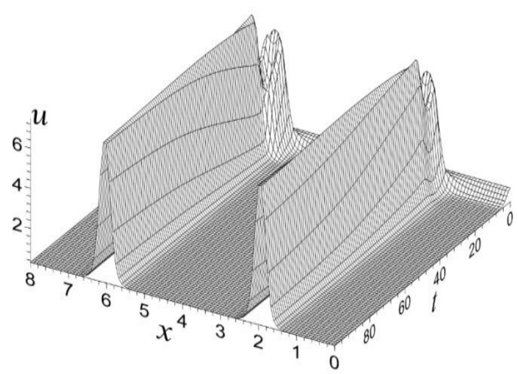

Fig. 2. Dynamics of variable u for $\alpha = 1.5$ (the Brusselator model)

With decreasing α without changing other parameters we can observe qualitative change of nonlinear dynamics of dissipative structures (fig. 3 for $\alpha = 1.3$, fig. 4 for $\alpha = 1.01$).

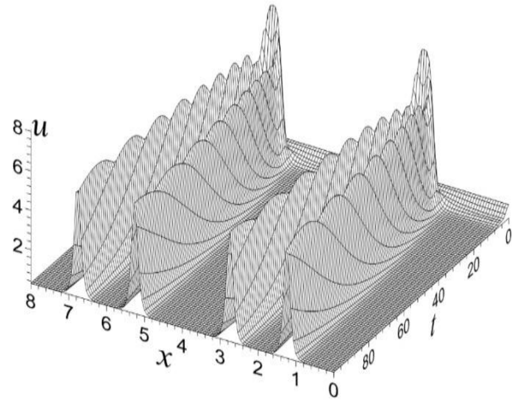

Fig. 3. Dynamics of variable u *for* $\alpha = 1.3$
(the Brusselator model)

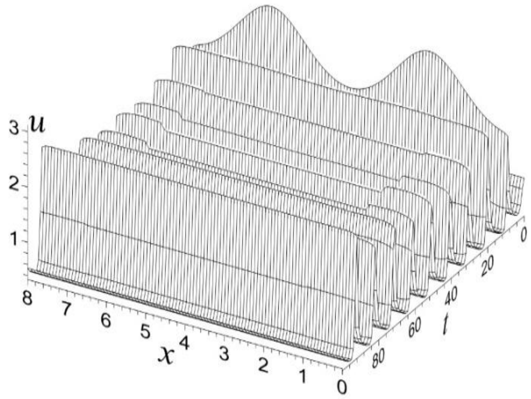

Fig. 4. Dynamics of variable u *for* $\alpha = 1.01$
(the Brusselator model)

Figs. 5 and 6 illustrate dissipative structures for the system (9), i.e. for the model with cubic nonlinearity for $A = -0.02$, $D_1 = 0.04$, $D_2 = 1$. Fig. 5 corresponds to the case of derivative of integer order $\alpha = 2$, while fig. 6 presents the results for fractional derivative of order $\alpha = 1.5$.

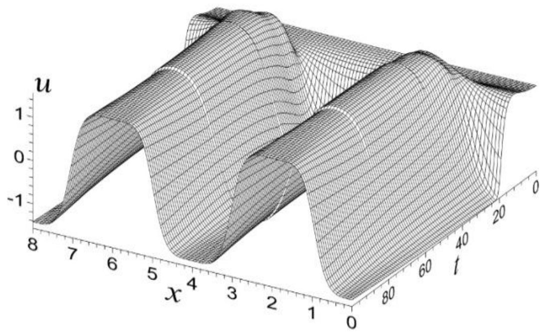

Fig. 5. Dynamics of variable u *for* $\alpha = 2$
(the model with cubic nonlinearity)

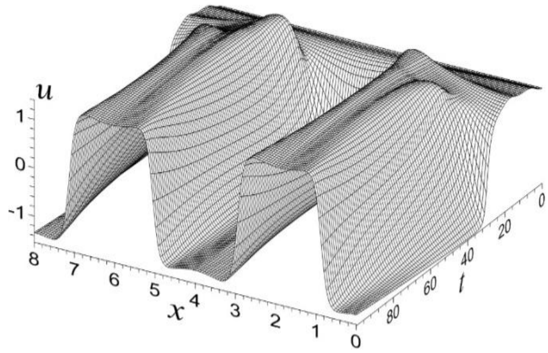

Fig. 6. Dynamics of variable u *for* $\alpha = 1.5$
(the model with cubic nonlinearity)

The decrease of α, in particular, for $\alpha = 1.2$ (fig. 7) and for the value close to unity $\alpha = 1.01$ (fig. 8) without changing other parameters, leads to qualitative change of dissipative structures.

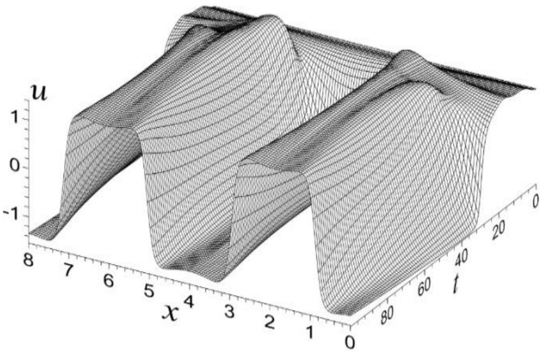

Fig. 7. Dynamics of variable u *for* $\alpha = 1.2$
(the model with cubic nonlinearity)

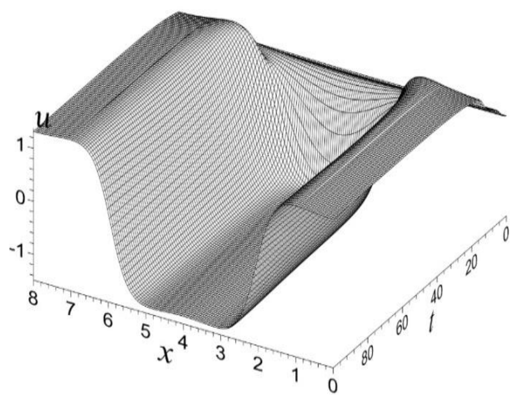

Fig. 8. Dynamics of variable u *for* $\alpha = 1.01$
(the model with cubic nonlinearity)

The obtained results of numerical simulations have been shown that decrease of order of fractional derivative, i.e. when the level of anomalous diffusion $\alpha < 2$ is essential, the qualitatively different types of spatio-temporal dynamics can occur in considered systems.

Conclusions

The nonlinear dynamics in generalized reaction-diffusion systems, namely in the Brusselator model and the model with cubic nonlinearity, in which the classical Laplacians are replaced by their fractional analogues, have been investigated. In these systems the fractional operator reflects the nonlocal behavior of superdiffusion. The linear stability analysis has been carried out. We have also determined the instability conditions of both Hopf and Turing.

We have obtained spatio-temporal patterns the occurrence of which is due to the properties of fractional operator of superdiffusion. It was shown that a decrease of order of fractional derivative i.e., when the level of anomalous diffusion is essential, the qualitatively different types of spatio-temporal nonlinear dynamics can occur in these systems. It was established, in particular, that the wave number depends on the order of fractional derivative.

The self-organization phenomena analyzed in this work can be used for studying nonlinear properties for a wide class of physical, chemical, biological, environmental and other active systems.

1. N. Fatin-Rouge, K. Starchev, J. Buffle, Size effects on diffusion processes within agarose gels, Biophys. J., 86 (2004), pp. 2710-2719. 2. T. Kosztołowicz, K. Dworecki, and St. Mrówczyński, How to Measure Subdiffusion Parameters, Phys. Rev. Lett., 94 (2005), 170602. 3. M. Weiss, Stabilizing Turing patterns with subdiffusion in systems with low particle numbers, Phys. Rev. E., 68 (2003), 036213. 4. F. D. A. Aarăo Reis and D. di Caprio, Crossover from anomalous to normal diffusion in porous media, Phys. Rev. E., 89 (2014), 062126. 5. J. M. Carcione, F. J. Sanchez-Sesma, F. Luzon, and J. J. P. Gavilan, Theory and simulation of time-fractional fluid diffusion in porous media, J. Phys. A: Math. Theor., 46 (2013), 345501. 6. S. Fomin, V. Chugunov, and T. Hashida, Mathematical modeling of anomalous diffusion in porous media, Fract. Different. Calc., 1, No 1.(2011), pp. 1-28. 7. J. Farago, H. Meyer, and A. N. Semenov, Anomalous Diffusion of a Polymer Chain in an Unentangled Melt, Phys. Rev. Lett., 107, Issue 17 (2011), 178301. 8. S. C. Weber, J. A. Theriot, A. J. Spakowitz, Subdiffusive motion of a polymer composed of subdiffusive monomers, Phys. Rev. E., 82 (2010), 011913. 9. R. Garra, Fractional-calculus model for temperature and pressure waves in fluid-saturated porous rocks, Phys. Rev. E., 84 (2011), 036605. 10. D. Roubinet, J.-R. de Dreuzy, D. M. Tartakovsky, Particle-tracking simulations of anomalous transport in hierarchically fractured rocks, Computers & Geosciences, 50 (2013), pp. 52-58. 11. B. A. Carreras, V. E. Lynch, and G. M. Zaslavsky, Anomalous diffusion and exit time distribution of particle tracers in plasma turbulence model, Phys. Plasmas, 8, Issue 12 (2001), pp. 5096-5103. 12. M. Priego, O. E. Garcia, V. Naulin, J. J. Rasmussen, Anomalous diffusion, clustering, and pinch of impurities in plasma edge turbulence, Phys. Plasmas, 12, Issue 6 (2005), 062312. 13. Y. Krivolapov, L. Levi, Sh. Fishman, M. Segev, and M. Wilkinson, Super-diffusion in optical realizations of Anderson localization, New J. Phys., 14 (2012), 043047. 14. E. Barkai, Y. Jung, R. Silbey, Theory of single-molucule spectroskopy: beyond the ensemble average, Annu. Rev. Phys. Chem., 55 (2004), pp. 457-507. 15. S. G. Samko, A. A. Kilbas, O. I. Marichev, Fractional integrals and derivatives, theory and applications, Gordon and Breach, Amsterdam, 1993 (Engl. Transl. from Russian, Nauka i Tekhnika, Minsk, 1987). 16. V. Uchaikin, Method of fractional derivatives, Artishok-Press, 2008 (in Russian). 17. I. Petras, Fractional-Order Nonlinear Systems. Modeling, Analysis and Simulation, Springer, 2011. 18. I. Podlubny, Fractional Differential Equations, San Diego: Acad. Press, 1999. 19. B. Y. Datsko , M. M. Gorak, Y. Y. Izmaylova, V. V. Meleshko, Dissipative structures in fractional reaction-diffusion systems, Appl. problems of mech. and math., 3 (2005), pp. 107-113. 20. V. Gafiychuk, B. Datsko, V. Meleshko, D. Blackmore, Analysis of the solutions of coupled nonlinear fractional reaction-diffusion equations, Chaos, Solitons and Fractals, 41, Issue 3 (2008), pp. 1095-1104. 21. B. Datsko, V. Gafiychuk, Complex nonlinear dynamics in subdiffusive activator-inhibitor systems, Communications in Nonlinear

Science and Numerical Simulation, 17, Issue 4 (2012), pp. 1673-1680. 22. A. A. Golovin, B. J. Matkowsky, and V. A. Volpert, Turing pattern formation in the Brusselator model with superdiffusion, J. Appl. Math., 69, No. 1 (2008), pp. 251-272. 23. G. Nicolis, I. Prigogine, Self-organization in Non-equilibrium Systems, Wiley, New York, 1977. 24. K .B. Oldham, J. Spanier, The Fractional Calculus: Theory and Applications of Differentiation and Integration to Arbitrary Order, New York: Acad. Press, 1974.