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Diffusion process modeling by using fractional-order models

Dominik Sierociuk [a], Tomas Skovranek [b,c], Michal Macias [a], Igor Podlubny [b], Ivo Petras [b,*], Andrzej Dzielinski [a], Pawel Ziubinski [a]

[a] Institute of Control and Industrial Electronics, Warsaw University of Technology, Koszykowa 75, 00-662 Warsaw, Poland
[b] Institute of Control and Informatization of Production Processes, BERG Faculty, Technical University of Košice, B. Němcovej 3, 042 00 Košice, Slovakia
[c] Biomedical Imaging Group, EPFL STI IMT LIB, Swiss Federal Institute of Technology Lausanne, CH-1015 Lausanne, Switzerland

A R T I C L E I N F O

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A B S T R A C T

This paper deals with a concept and description of a RC network as an electro-analog model of diffusion process which enables to simulate heat dissipation under different initial and boundary conditions. It is based on well-known analogy between heat and electrical conduction. In the paper are compared analytical solution together with numerical solution and experimentally measured data. For the first time a fractional order model of diffusion process and its modeling via lumped RC network has been used. Simple examples of simulations, measurements and their comparison are shown.

1. Introduction

Fractional calculus and fractional differential equations have been used in various areas of the applications, for instance bioengineering [4], physics [2,23], chaos theory [11], viscoelasticity [5], control system engineering [1,7,13,22], fractional signal processing techniques [18] and many others areas (see e.g. [8,10,17]). One of the another important area of applications is the electrical engineering.

This article describes how to model diffusion using a RC network as an electro-analog model of diffusion process. Paper is based on well-known analogy between heat and electrical conduction. Such approach was already used for modeling the diffusion process described by integer-order differential equation [3]. In this article a fractional-order model of the diffusion process and its modeling via RC network is used. Experimentally obtained results are compared with analytical and numerical solution of the fractional order diffusion equation. For numerical computation of the fractional-order partial differential equation a matrix approach has been used [15,16].

2. Fractional calculus

Fractional order differential calculus is a generalization of integer order integral and derivative to real or even complex order. This idea has first emerged at the end of 17th century, and has been developed in the area of mathematics throughout 18th and 19th century in the works of e.g. Liouville, Riemann, Cauchy, Abel, Grünwald and many others. More recently, by the end of 20th century, it turned out that some physical phenomena are modeled more accurately when fractional calculus is in use. There exist two (in fact three) main definitions of the fractional order integrals, derivatives and differences: Riemann–Liouville, Caputo, and Grünwald–Letnikov [6,8,10,13]. Some other, are also present in literature, but less

* Corresponding author.
E-mail address: ivo.petras@tuke.sk (I. Petras).

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commonly used in the applications. To be precise, the Riemann–Liouville and Caputo definitions concern both fractional derivative and integral.

To define the fractional order differ-integral, the definition of the $\Gamma(x)$ function is needed. The $\Gamma(x)$ function is given in the following way [13]:

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt, \tag{1}$$

where $\Re(x) > 0$.

In this article we will consider the Caputo's definition, which can be written as [13]:

$${}_0D_t^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{f^{(n)}(\tau)}{(t-\tau)^{\alpha-n+1}} d\tau, \tag{2}$$

for $n-1 < \alpha < n$. The initial conditions for the fractional order differential equations with the Caputo derivatives are in the same form as for the integer-order differential equations. For the Caputo partial fractional derivative of order α of a function $f(t,\lambda)$ with respect to variable t we will use the notation of the form $\partial^\alpha f(t,\lambda)/\partial t^\alpha$, which is often used in the related literature.

The Laplace transform method is used often for solving engineering problems. The formula for the Laplace transform of the Caputo fractional derivative (2) has the form [13]:

$$\int_0^\infty e^{-st} {}_0D_t^\alpha f(t) dt = s^\alpha F(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0) \tag{3}$$

for $n-1 < \alpha \leqslant n$, where $s \in \mathbb{C}$ denotes the Laplace operator, and $\mathbb{C}$ denotes a set of complex numbers.

3. Description of diffusion process

One of a good example of diffusion process is a heat transfer action, when a heat (energy, temperature) is transported through a material. The description of such a processes can be meet in Sierociuk et al. [19]. Let us assume the heat transfer process in semi-infinite beam, with respect to the temperature (we will be able to control temperature at the beginning of the beam and observe also temperature at each point of the beam). The analog equivalent of this process is a transmission line presented in Fig. 1. The voltage in each stage of RC-line represents a temperature in heat transfer process, and similarly the current represents a heat flux.

From the analog model the diffusion equation can be obtained very shortly. The voltage between two stages is a voltage on the resistor, and is proportional to the current in this stage. This can be written as follows:

$$u(x,t) - u(x+dx,t) = Ri(x,t) \tag{4}$$

what, in limit for $dx \to 0$, can be rewritten as

$$\frac{\partial}{\partial x} u(x,t) = Ri(x,t) \tag{5}$$

Similar, the voltage of the capacitor in each stage can be described

$$i(x,t) - i(x+dx,t) = C\frac{\partial}{\partial t} u(x,t) \tag{6}$$

what, in limit for $dx \to 0$, can be rewritten as

$$\frac{\partial}{\partial x} i(x,t) = C\frac{\partial}{\partial t} u(x,t) \tag{7}$$

This two equations (for resistor and capacitor) can be written together in the form of diffusion equation:

$$\frac{\partial^2}{\partial x^2} u(x,t) = RC\frac{\partial}{\partial t} u(x,t) \tag{8}$$

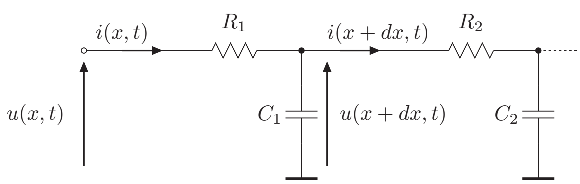

Fig. 1. Scheme of transmission line.

3.1. Evaluation of diffusion process equation

For a case of the ideal heating process, without energy loss, of a semi-infinite beam that equation can be written in the following form

$$\frac{\partial}{\partial t}T(t,\lambda) = \frac{1}{a^2}\frac{\partial^2 T(t,\lambda)}{\partial \lambda^2}, \tag{9}$$

with the following boundary conditions:

$$T(0,\lambda) = 0, \quad T(t,0) = u(t), \tag{10}$$

where $T(t,\lambda)$ is a temperature of the beam at time instant t and space coordinate (distance) λ, and $\frac{1}{a^2}$ is a beam material conductivity.

As it was presented in Podlubny and Sierociuk et al. [13,19] the following relation between the heat flux and the temperature at the desired point holds (it can be obtained during solving the Eq. (9) in Laplace domain):

$$H(t,\lambda) = \frac{1}{a}\frac{\partial^{0.5}}{\partial t^{0.5}}T(t,\lambda). \tag{11}$$

Analytical solution for $T(s,0) = c1(t)$ and $\alpha = 1$ is

$$T(t,\lambda_1) = c\,\mathrm{erfc}\left(\frac{\lambda_1 a}{2\sqrt{t}}\right) \tag{12}$$

3.2. Evaluation of diffusion process equation for loss case

Let as assume the situation that in each point of diffusive material length a part of the heat flux is dissipated. Moreover, the value of this dissipation flux is proportional to the temperature of this point. In order to achieve it, let us expand the Eq. (11), in the same way as in Sierociuk et al. [19], into the following form:

$$\frac{\partial}{\partial \lambda}H(t,\lambda) = \frac{1}{a}\frac{\partial^{0.5}}{\partial t^{0.5}}H(t,\lambda) + bH(t,\lambda), \tag{13}$$

where a is the same beam material conductivity as for ideal diffusion case and, b is a coefficient of heat flux dissipation.

This can be expressed as the analog model presented in Fig. 2, where losing of heat flux is represented by additional resistors connected parallel to capacitors.

The diffusion equation, in this case, has the following form

$$\frac{\partial^2}{\partial \lambda^2}T(t,\lambda) = a^2\frac{\partial}{\partial t}T(t,\lambda) + 2a^3 b\frac{\partial^{0.5}}{\partial t^{0.5}}T(t,\lambda) + a^4 b^2 T(t,\lambda) \tag{14}$$

Solution of this equation in Laplace domain has the following form

$$T(s,\lambda_1) = e^{-\lambda_1\left(as^{0.5}+a^2 b\right)}T(s,0). \tag{15}$$

what can be rewritten as

$$T(s,\lambda_1) = e^{-\lambda_1 a^2 b}e^{-\lambda_1 a s^{0.5}}T(s,0). \tag{16}$$

Analytical solution for $T(s,0) = c1(t)$ and $\alpha = 1$ is

$$T(t,\lambda_1) = ce^{-\lambda_1 a^2 b}\mathrm{erfc}\left(\frac{\lambda_1 a}{2\sqrt{t}}\right) \tag{17}$$

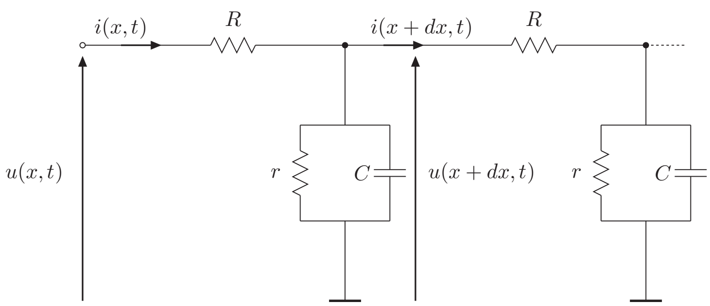

Fig. 2. Scheme of transmission line with heat dissipation.

4. Matrix approach for solving fractional order diffusion equations

This approach is based on the fact that operation of the fractional calculus can be expressed by matrix [16]. It follows from Podlubny [14], that the left-sided Riemann–Liouville or Caputo fractional derivative $v^{(\alpha)}(t) = {}_0D_t^{\alpha}v(t)$ can be approximated in all nodes of the equidistant discretization net $t = j\tau$ $(j = 0, 1, \dots, n)$ simultaneously with the help of the upper triangular strip matrix $B_n^{(\alpha)}$ as:

$$\left[v_n^{(\alpha)}\ v_{n-1}^{(\alpha)}\ \dots\ v_1^{(\alpha)}\ v_0^{(\alpha)}\right]^T = B_n^{(\alpha)}[v_n\ v_{n-1}\ \dots\ v_1\ v_0]^T, \tag{18}$$

where

$$B_n^{(\alpha)} = \frac{1}{\tau^{\alpha}}\begin{bmatrix} \omega_0^{(\alpha)} & \omega_1^{(\alpha)} & \ddots & \ddots & \omega_{n-1}^{(\alpha)} & \omega_n^{(\alpha)} \\ 0 & \omega_0^{(\alpha)} & \omega_1^{(\alpha)} & \ddots & \ddots & \omega_{n-1}^{(\alpha)} \\ 0 & 0 & \omega_0^{(\alpha)} & \omega_1^{(\alpha)} & \ddots & \ddots \\ \dots & \dots & \dots & \ddots & \ddots & \ddots \\ 0 & \dots & 0 & 0 & \omega_0^{(\alpha)} & \omega_1^{(\alpha)} \\ 0 & 0 & \dots & 0 & 0 & \omega_0^{(\alpha)} \end{bmatrix} \tag{19}$$

$$\omega_j^{(\alpha)} = (-1)^j\binom{\alpha}{j}, \quad j = 0, 1, \dots, n. \tag{20}$$

Similarly, the right-sided Riemann–Liouville or Caputo fractional derivative $v^{(\alpha)}(t)={}_tD_b^{\alpha}v(t)$ can be approximated in all nodes of the equidistant discretization net $t = j\tau$ $(j = 0, 1, \dots, n)$ simultaneously with the help of the lower triangular strip matrix $F_n^{(\alpha)}$:

$$\left[v_n^{(\alpha)}\ v_{n-1}^{(\alpha)}\ \dots\ v_1^{(\alpha)}\ v_0^{(\alpha)}\right]^T = F_n^{(\alpha)}[v_n\ v_{n-1}\ \dots\ v_1\ v_0]^T \tag{21}$$

$$F_n^{(\alpha)} = \frac{1}{\tau^{\alpha}}\begin{bmatrix} \omega_0^{(\alpha)} & 0 & 0 & 0 & \dots & 0 \\ \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & 0 & \dots & 0 \\ \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & \dots & 0 \\ \ddots & \ddots & \ddots & \ddots & \dots & \dots \\ \omega_{n-1}^{(\alpha)} & \ddots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 \\ \omega_n^{(\alpha)} & \omega_{n-1}^{(\alpha)} & \ddots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} \end{bmatrix} \tag{22}$$

The symmetric Riesz derivative of order β can be approximated based on its definition as a combination of the approximations (18) and (21) for the left and right-sided Riemann–Liouville derivatives, or using the centered fractional differences approximation of the symmetric Riesz derivative suggested recently by Ortigueira [9]. The general formula is the same:

$$\left[v_m^{(\beta)}\ v_{m-1}^{(\beta)}\ \dots\ v_1^{(\beta)}\ v_0^{(\beta)}\right]^T = R_m^{(\beta)}[v_m\ v_{m-1}\ \dots\ v_1\ v_0]^T \tag{23}$$

In the first case, the approximation for the left-sided Caputo derivative is taken one step ahead, and the approximation for the right-sided Caputo derivative is taken one step back. This leads to the matrix

$$R_m^{(\beta)} = \frac{h^{-\alpha}}{2}[{}_{-1}U_m + {}_{+1}U_m] \tag{24}$$

In the second case (Ortigueira's definition) we have the following symmetric matrix:

$$R_m^{(\beta)} = h^{-\beta}\begin{bmatrix} \omega_0^{(\beta)} & \omega_1^{(\beta)} & \omega_2^{(\beta)} & \omega_3^{(\beta)} & \dots & \omega_m^{(\beta)} \\ \omega_1^{(\beta)} & \omega_0^{(\beta)} & \omega_1^{(\beta)} & \omega_2^{(\beta)} & \dots & \omega_{m-1}^{(\beta)} \\ \omega_2^{(\beta)} & \omega_1^{(\beta)} & \omega_0^{(\beta)} & \omega_1^{(\beta)} & \dots & \omega_{m-2}^{(\beta)} \\ \ddots & \ddots & \ddots & \ddots & \dots & \dots \\ \omega_{m-1}^{(\beta)} & \ddots & \omega_2^{(\beta)} & \omega_1^{(\beta)} & \omega_0^{(\beta)} & \omega_1^{(\beta)} \\ \omega_m^{(\beta)} & \omega_{m-1}^{(\beta)} & \ddots & \omega_2^{(\beta)} & \omega_1^{(\beta)} & \omega_0^{(\beta)} \end{bmatrix} \tag{25}$$

$$\omega_k^{(\beta)} = \frac{(-1)^k \Gamma(\beta+1)\cos(\beta\pi/2)}{\Gamma(\beta/2-k+1)\Gamma(\beta/2+k+1)}, \quad k = 0, 1, \ldots, m. \tag{26}$$

Both these approximations of symmetric Riesz derivatives give practically the same numerical results and in case of numerical solution of partial fractional differential equations lead to a well-posed matrix of the resulting algebraic system.

Similarly, if in addition to fractional-order time derivative we also consider symmetric fractional-order spatial derivatives, then we have to use all nodes at the considered time layer from the leftmost to the rightmost spatial discretization node.

Let us consider the nodes $(ih, j\tau),\ j = 0, 1, 2, \ldots, n$, corresponding to all time layers at ith spatial discretization node. It has been shown in Podlubny [14] that all values of αth order time derivative of $u(x,t)$ at these nodes are approximated using the discrete analogue of differentiation of arbitrary order:

$$\left[u_{i,n}^{(\alpha)}\ u_{i,n-1}^{(\alpha)}\ \ldots\ u_{i,2}^{(\alpha)}\ u_{i,1}^{(\alpha)}\ u_{i,0}^{(\alpha)}\right] = B_n^{(\alpha)} \left[u_{i,n}\ u_{i,n-1}\ \ldots\ u_{i,2}\ u_{i,1}\ u_{i,0}\right]^T. \tag{27}$$

In order to obtain a simultaneous approximation of αth order time derivative of $u(x,t)$ in all nodes, we need to arrange all function values u_{ij} at the discretization nodes to the form of a column vector $u_{nm} = [\ldots]^T$, which has the structure described in Podlubny et al. [16].

In visual terms, we first take the nodes of nth time layer, then the nodes of $(n-1)$th time layer, and so forth, and put them in this order in a vertical column stack.

The matrix that transforms the vector U_{nm} to the vector $U_t^{(\alpha)}$ of the partial fractional derivative of order α with respect to time variable can be obtained as a Kronecker product of the matrix $B_n^{(\alpha)}$, which corresponds to the fractional ordinary derivative of order α (recall that n is the number of time steps), and the unit matrix E_m (recall that m is the number of spatial discretization nodes):

$$T_{mn}^{(\alpha)} = B_n^{(\alpha)} \otimes E_m \tag{28}$$

Similarly, the matrix that transforms the vector U to the vector $U_x^{(\beta)}$ of the partial fractional derivative of order β with respect to spatial variable can be obtained as a Kronecker product of the unit matrix E_n (recall that m is the number of spatial discretization nodes), and the matrix $R_m^{(\beta)}$, which corresponds to a symmetric Riesz ordinary derivative of order β [9], (recall that m is the number of time steps):

$$S_{mn}^{(\alpha)} = E_n \otimes R_m^{(\beta)}. \tag{29}$$

Having these approximations for partial fractional derivatives with respect to both variables, we can immediately discretize the general form of the fractional diffusion equation by simply replacing the derivatives with their discrete analogs. Namely, the equation

$${}_0^C D_t^{\alpha} u - \chi \frac{\partial^{\beta} u}{\partial |x|^{\beta}} = f(x,t) \tag{30}$$

is discretized as

$$\left\{ B_n^{(\alpha)} \otimes E_m - \chi E_n \otimes R_m^{(\beta)} \right\} u_{nm} = f_{nm}. \tag{31}$$

In the case of diffusion process with heat flux dissipation, the Eq. (14) can be rewritten into general discrete form using the Podlubny's matrix approach as

$$\left\{ \chi_1 B_n^{(\alpha)} \otimes E_m + \chi_2 B_n^{(\beta)} \otimes E_m + \chi_3 I_n \otimes E_m - E_n \otimes R_m^{(\gamma)} \right\} u_{nm} = f_{nm}. \tag{32}$$

Initial and boundary conditions must be equal to zero. If it is not so, then an auxiliary unknown function must be introduced, which satisfies the zero initial and boundary conditions. In this way, the non-zero initial and boundary conditions moves to the right-hand side of the equation for the new unknown function.

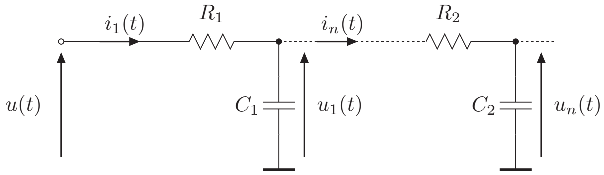

Fig. 3. Analog model of diffusion process with heat dissipation.

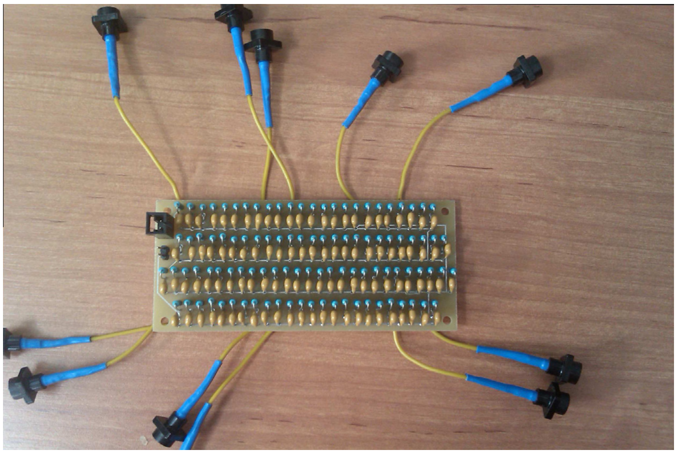

Fig. 4. A circuit board of the diffusion process with heat dissipation.

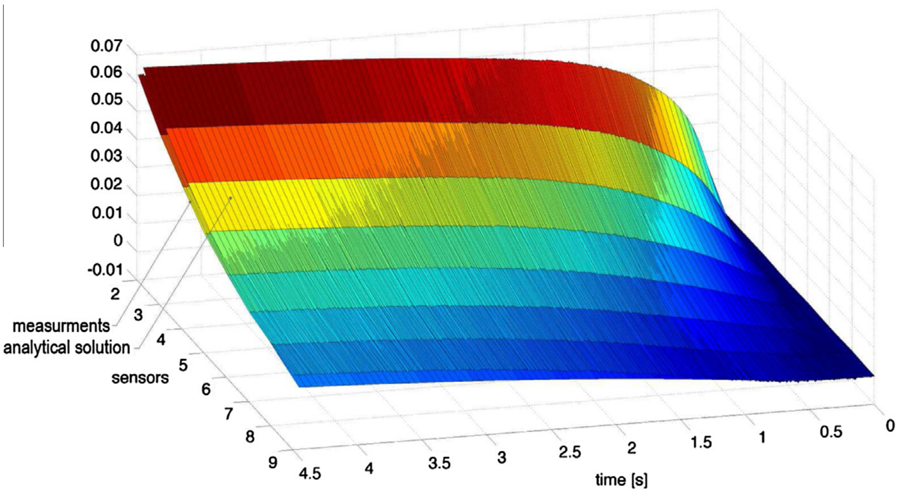

Fig. 5. Comparison of analog modeling and analytical solution.

Table 1
The squared error for diffusion process with heat flux dissipation. The bold font in the Table stays for the sum of errors for all sensors.

	Analog vs. analytical	Analog vs. numerical	Analytical vs. numerical
Sensor 2	1.0524e – 04	1.1270e – 04	16.0752e – 07
Sensor 3	2.6270e – 04	2.6622e – 04	6.3378e – 07
Sensor 4	4.9037e – 04	4.8290e – 04	15.6129e – 07
Sensor 5	7.0636e – 04	6.9736e – 04	10.7388e – 07
Sensor 6	9.1195e – 04	9.1108e – 04	9.8623e – 07
Sensor 7	13.4889e – 04	13.7164e – 04	13.6162e – 07
Sensor 8	17.3842e – 04	18.0666e – 04	24.9588e – 07
Sensor 9	22.3321e – 04	23.8260e – 04	51.8428e – 07
Sensor 10	28.4296e – 04	31.2802e – 04	110.4091e – 07
Sensor 11	39.1501e – 04	44.4508e – 04	232.4328e – 07
Sensor 12	7.9172e – 04	9.2346e – 04	479.2257e – 07
$\sum$**error**	**153.4682e – 04**	**165.2770e – 04**	**.9711e – 04**

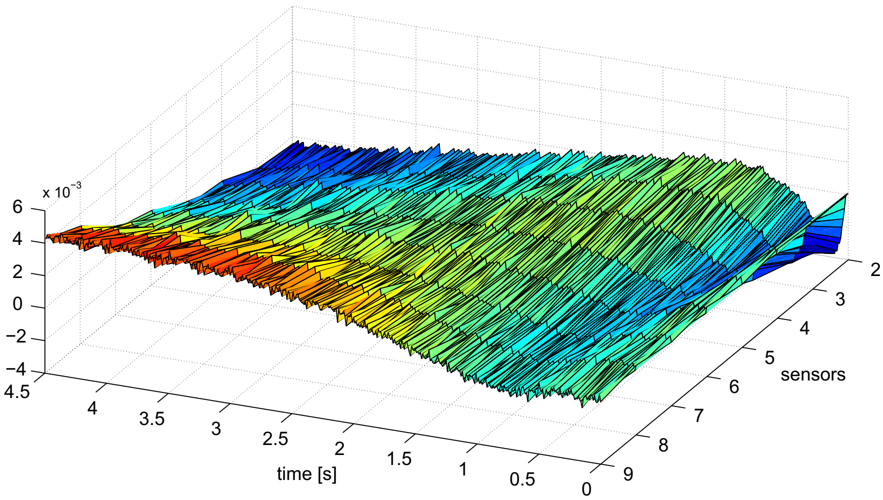

Fig. 6. Error between analog modeling and analytical solution.

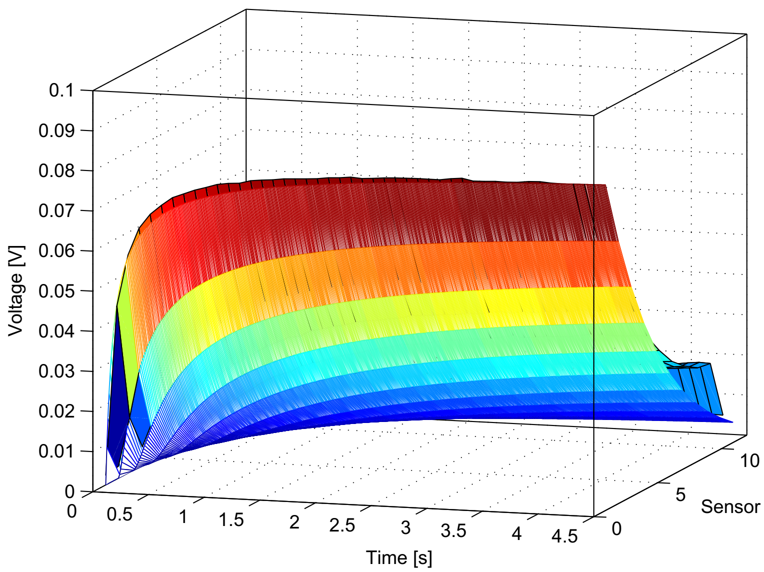

Fig. 7. Comparison of analog modeling and numerical solution.

5. Results of diffusion process modeling using three different representations

In this section the data originating from physical system for diffusion process with dissipation are compared with the results obtained using analytical and numerical models.

Experimental setup is based on analog model of diffusion process with heat dissipation shown in Fig. 3, the analytical solution is presented in Section 3 and the numerical algorithm is presented in Section 4.

5.1. Experimental setup of the electrical circuit

In general the analog model of diffusion process is based on half order impedance implementation studied in Refs. [12,20,21]. It contains 200 elements and was designed and made according to the scheme presented in Fig. 3 with the following values of the passive elements: $R_1 = 2.4\ \text{k}\Omega$, $R_2 = 8.2\ \text{k}\Omega$, $C_1 = 330$ nF and $C_2 = 220$ nF. Due to decrease a noise ratio of the dSPACE A/D converters, which improve the accuracy of dSPACE card analog inputs, their input resistance was slightly reduced and comparable with resistors used in analog diffusion model. In this fact, when the voltages $u_1, \ldots, u_n$ from Fig. 3 are directly connected to cards' inputs the setup stays a diffusion process with dissipation.

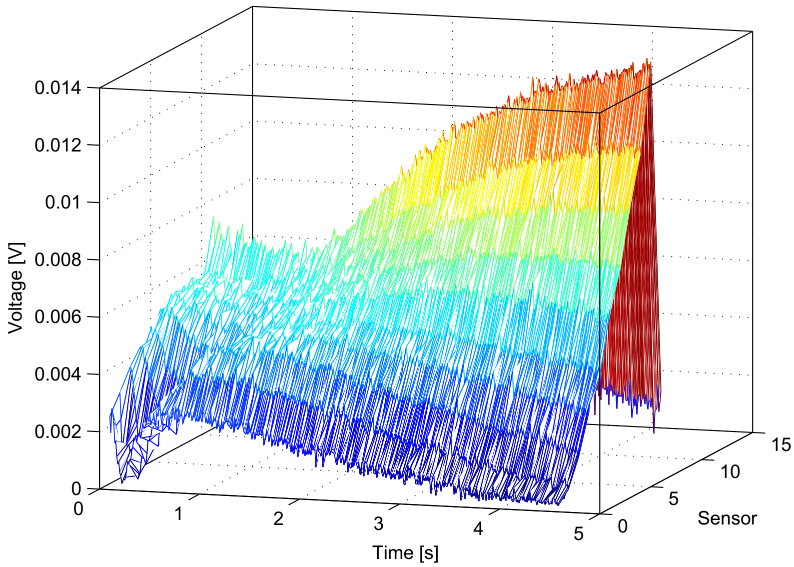

Fig. 8. Error between analog modeling and numerical solution.

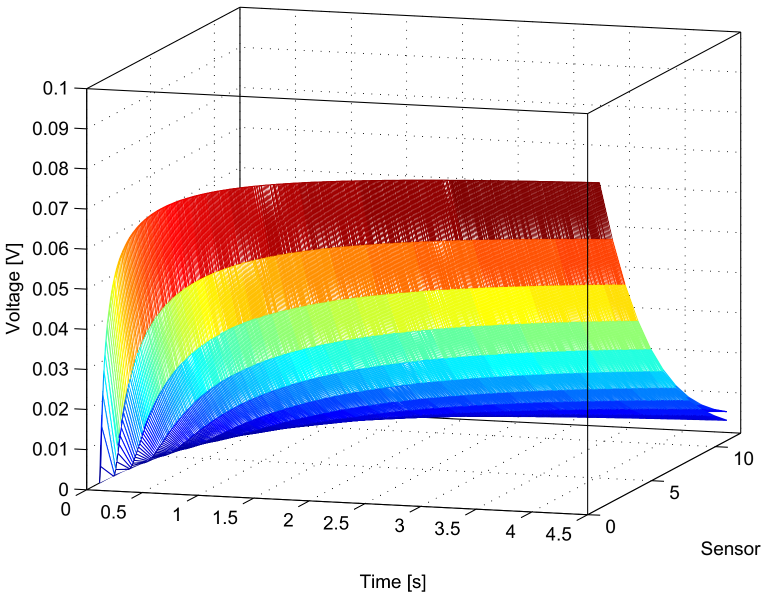

Fig. 9. Comparison of analytical and numerical solutions.

The experimental setup contains:

1. dSPACE DS1104 PPC card mounted in PC,
2. electrical circuit – the analog model of the diffusion process.

The experimental data were gathered by sensors connected to every 8th node of the analog model. To clarify the first voltage the sensors were placed into the input circuit terminals, the next measurement were gathered by second sensor (ADC channel) connected to the 8th node of domino ladder structure, and next sensors were connected to each next 8th node (e.g. $16, 24, \ldots$).

The overview of the circuit boards for diffusion process with dissipation is presented in Fig. 4.

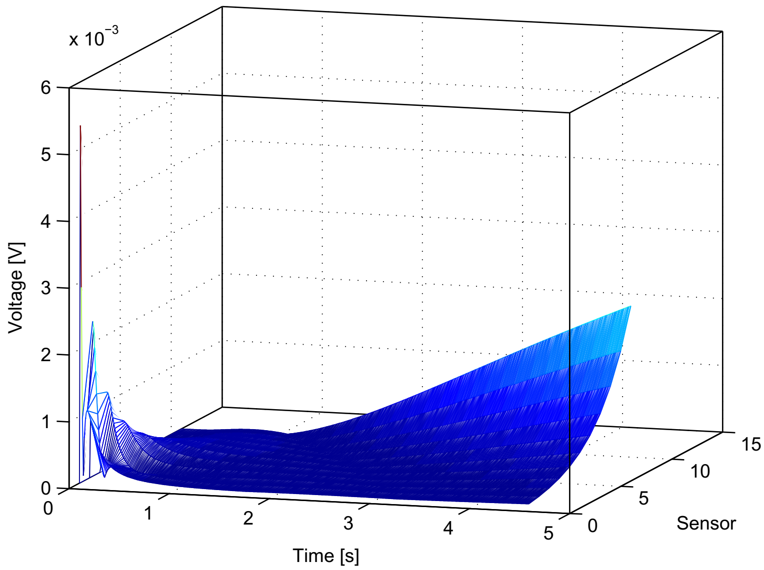

Fig. 10. Error between analytical and numerical solutions.

5.2. Comparison of the results of analog, analytical and numerical representations of diffusion process with dissipation

Results of analog modeling for diffusion process with dissipation were collected based on the experimental system presented in Figs. 3 (scheme) and 4 (real view). Based on numerical minimization of square error between experimental data and analytical solution, given by Eq. (17), the following parameters were obtained:

$$a = 0.281073708524755; \quad b = 1.674579293537321; \tag{33}$$

Due to used numerical algorithm, the identified parameters were obtained for minimization error for 3th–8th sensors.

Experimental data for diffusion process with dissipation, for sensors 1–11 and its comparison to the analytical solution given by Eq. (17), using identified parameters a and b, are presented in Fig. 5 and Table 1. The modeling error for analog and analytical results is presented in Fig. 6.

For numerical solution the model Eq. (14) was evaluated, and the fractional derivatives were calculated using the Podlubny's matrix approach. It was written in the discrete form Eq. (32), where the used parameters were $\alpha = 1,\ \beta = 1/2,\ \chi_1 = a^2,\ \chi_2 = 2a^3b,\ \chi_3 = a^4b^2$. The numerical results were compared to the analog samples, shown in Fig. 7 (the smooth surface in the front is representing the numerical solution and the measured samples are represented by the grid surface behind), as well as to the analytical model Fig. 9 (numerical solution in the front, analytical solution behind). The error surfaces for all the comparisons of different approaches for describing heat transfer can be found in Figs. 6, 8, 10, respectively.

The full list of least squared errors between the measured analog samples, analytical solution and numerical solution of the diffusion process with heat flux dissipation can be found in Table 1, where again the error for each sensor as well as the total error is given.

As it can be seen the error between analog and analytical results at the beginning of the plots is very limited and increase with the time and number of sensors. It is caused by the fact, that analytical solution is obtained for an assumption that the diffusion media (e.g. the heating beam) is infinite. The analog realization has only finite length, what has an effect in the dynamics of the system, the finite length domino ladder can be charged faster that infinite one. This can be observed at the point that the voltage value start to be constant when the analytical model still increase this value.

For the case of comparison between numerical and analytical solutions we can recognize that both solutions are very close. It confirms correctness of used matrix approach for solving such a type of fractional order partial differential equations.

6. Conclusions

The paper presents detailed formulation of diffusion process with dissipation and its description in the form of fractional order partial differential equation. For heat transfer case the diffusion with dissipation occurs when a part of the heat flux dissipate to environment in the whole length of the beam, what can be met when the beam is not ideally insulated from the environment. The realization of such a process was given also in the form of analog circuit and numerical algorithm. The analog model of diffusion equation was build based on modified domino ladder approximation of half order impedance. Numerical solution was obtained based on matrix approach for fractional order partial differential equations. The experimentally obtained results were compared with analytical and numerical solution, both based on fractional calculus and numerical solution. Comparison of results confirm high accuracy of used methods and important differences between used approach. The analytical and numerical solution are very close and can describe an infinite length case, while analog realization could describe only finite length case. The results presented in this paper allows to better understand the diffusion process with (heat flux, current) dissipation and its analog and numerical realizations.

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