Applied Mathematics and Computation 257 (2015) 365–373

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Heat conduction modeling by using fractional-order derivatives ☆

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ARTICLE INFO

Keywords:
Fourier heat conduction equation
Heat conduction
Analytical and numerical methods
Derivatives of integer- and fractional-order

ABSTRACT

The article deals with the heat conduction modeling. A brief historical overview of the authors who have dealt with the heat conduction and overview of solving methods is listed in the introduction of article. In the next section a mathematical model of one-dimensional heat conduction with using derivatives of integer- and fractional-order is described. The methods of solving models of heat conduction are described, namely analytical and numerical methods. In the case of numerical methods regards the finite difference method by using Grünwald–Letnikov definition for the fractional time derivative. Implementation of these individual methods was realized in MATLAB. The two libraries of *m*-functions for the heat conduction model have been created, namely Heat Conduction Toolbox and Fractional Heat Conduction Toolbox. At the conclusion of the article the simulations examples with using toolboxes are listed.

1. Introduction

Heat conduction process, described by partial differential equation, was first formulated by Jean Baptiste Joseph Fourier (1768–1830). In 1807 he wrote an article "Partial differential equation for heat conduction in solids". The issue of heat conduction was addressed by other scientists as well, such as Fick, Maxwell, Einstein, Richards, Taylor [1].

The various analytical and numerical methods are used to the solution the Fourier heat conduction equation [2,3]. In the case of heat conduction in materials with non-standard structure, such as polymers, granular and porous materials, composite materials and so on, a standard description is insufficient and required the creation of more adequate models with using derivatives of fractional-order [4–8]. The causes are mainly memory systems and ongoing processes [9–13], roughness or porosity of the material [14–16] and also fractality and chaotic behavior of systems [17–26].

The issue of research and development methods and tools for processes modeling with using fractional-order derivatives is very actual, since it means a qualitatively new level of modeling. Important authors of the first articles were Fourier, Abel, Leibniz, Grünwald and Letnikov. Mathematicians like Liouville (1809–1882) [27,28] and Riemann (1826–1866) [29] made major contributions to the theory of fractional calculus.

Nowadays there are a number of analytical [30–37] and numerical solutions of fractional heat conduction equation. In the case of numerical methods are developed different methods based on the random walk models [38–41], the finite difference

☆ This work was supported by the Slovak Research and Development Agency under the contract No. APVV-0482-11 and by projects VEGA 1/0729/12, 1/0552/14, and 1/0529/15.

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http://dx.doi.org/10.1016/j.amc.2014.12.136
0096-3003/

method (FDM) [42–44], the finite element method [45–48], numerical quadrature [49–51], the method of Adomian decomposition [52,53], Monte Carlo simulation [54,55], matrix approach [4,5,56] or the matrix transform method [57,58]. The finite difference method is an extended method where are used an explicit [42,59,60], an implicit [43,61–63], and a Crank–Nicolson scheme [44,64]. For the Crank–Nicolson scheme, the literature describes the use of Grünwald–Letnikov definition only for a spatial derivative [62,65–67].

The work presented in this article is mainly aimed at the implementation of FDM for the fractional heat conduction equation in MATLAB and in the case of Crank–Nicolson scheme brings the use of Grünwald–Letnikov definition for the time derivative. The article does not address the questions of the stability and convergency because they are described in detail in many works, e.g. [60,63,68].

2. Heat conduction models

A heat conduction is a molecular transfer of thermal energy in solids, liquids and gases due to the temperature difference. The process of the heat conduction takes place between the particles of the substance when they directly touch each-other and have different temperature. Existing models of heat conduction processes are divided according to various criterions. We consider a division into two groups to models with using derivatives of integer and fractional order.

2.1. Models with using derivatives of integer order

Models with using derivatives of integer order are the non-stationary and stationary models. Non-stationary models are described by Fourier heat conduction equation, where the temperature T (K) is a function of spatial coordinate x (m) and time τ (s). In the case of one-dimensional heat conduction it has the following form

$$\begin{aligned} &\frac{\partial T(x,\tau)}{\partial \tau} = \left(\sqrt{a}\right)^2 \frac{\partial^2 T(x,\tau)}{\partial x^2} \quad \text{for} \quad 0 < x < L \quad \text{and} \quad \tau > 0, \\ &T(0,\tau) = T_1, \quad T(L,\tau) = T_2 \quad \text{for} \quad \tau > 0, \\ &T(x,0) = f(x) \quad \text{for} \quad 0 \leqslant x \leqslant L, \end{aligned} \tag{1}$$

where $a = \lambda/(\rho \cdot c_p)$ is thermal diffusivity ($m^2\ s^{-1}$), ρ is density ($kg\ m^{-3}$), c_p is specific heat capacity ($J\ kg^{-1}\ K^{-1}$) and λ is thermal conductivity ($W\ m^{-1}\ K^{-1}$).

2.2. Models with using derivatives of fractional order

A more general formulation of the task for modeling not only one-dimensional heat conduction is based on the model in which on the left-hand side of the Eq. (1) instead of the first derivative with respect to time, the derivative of order α occurs, i.e. we can find it in the form

$$\begin{aligned} &\frac{\partial^\alpha T(x,\tau)}{\partial \tau^\alpha} = (b)^2 \frac{\partial^2 T(x,\tau)}{\partial x^2} \quad \text{for} \quad 0 < x < L \quad \text{and} \quad \tau > 0, \\ &T(0,\tau) = T_1, \quad T(L,\tau) = T_2 \quad \text{for} \quad \tau > 0, \\ &T(x,0) = f(x) \quad \text{for} \quad 0 \leqslant x \leqslant L, \end{aligned} \tag{2}$$

where b represents a constant coefficient with the unit $m{\cdot}s^{-\alpha/2}$.

3. Methods of solution

Methods used to solve models (1) and (2) are divided into *analytical methods* and *numerical methods*.

3.1. Analytical methods

Analytical methods can be used for solving problems in a bounded, semi-bounded or unbounded interval. Analytical solution of heat conduction model (1) for a bounded interval $\langle 0, L\rangle$ is given by the following function, which corresponds to the sum of the product of trigonometric and exponential functions

$$T(x,\tau) = \sum_{k=1}^{\infty} \left[c_k\ e^{-(n\sqrt{a})^2 \tau} \sin nx \right] + \frac{1}{L}(T_2 - T_1)x + T_1, \tag{3}$$

where

$$c_k = \frac{2}{L} \int_0^L \left[f(\xi) - \frac{1}{L}(T_2 - T_1)\xi - T_1 \right] \sin \frac{k\pi\xi}{L} d\xi. \tag{4}$$

Analytical solution for a fractional diffusion-wave equation or model (2) can be described by the following relation, which includes also the solution (1) and thus represents a more general form of analytical solution [31]

$$T(x,\tau)=\sum_{k=1}^{\infty}\left[c_k\,E_\alpha\left(-(nb)^2\tau^\alpha\right)\sin nx\right]+\frac{1}{L}(T_2-T_1)x+T_1, \tag{5}$$

where $E_\alpha(z)$ is the Mittag–Leffler function, e.g. $E_1(-z)=e^{-z}$, resp. $E_2(-z^2)=\cos(z)$, α is the order of fractional derivative.

In the case that we would like to consider different initial conditions, for example in the form of constant values, possibly in a linear or quadratic shape, then it is appropriate to choose the initial condition in the form of a polynomial of second order $f(\xi)=a_0+a_1\xi+a_2\xi^2$. For a given shape of the function the form of c_k was subsequently derived as follows

$$c_k=\frac{2}{nL}\left[T_2-a_0-a_1L+a_2\left(\frac{2}{n^2}-L^2\right)\right](-1)^k-T_1+a_0-a_2\frac{2}{n^2}, \tag{6}$$

where $n=k\pi/L$.

3.2. Numerical methods

The most famous numerical method for solving models (1) and (2) is FDM with explicit, implicit and Crank–Nicolson scheme.

3.2.1. Explicit scheme

The temperature in a new time step T_{p+1} is calculated from the three temperatures at positions $m-1$, $m+1$ and m in the previous time step (Fig. 1(a)). Explicit scheme for solving the heat conduction model defined by Eq. (1) in the case of homogeneous material has the following form

$$T_{m,p}=MT_{m-1,p-1}+T_{m,p-1}-2MT_{m,p-1}+MT_{m+1,p-1} \tag{7}$$

and in the case of non-homogeneous material has the form

$$T_{m,p}=M_{m-1}T_{m-1,p-1}+T_{m,p-1}-(M_{m-1}+M_m)T_{m,p-1}+M_mT_{m+1,p-1}, \tag{8}$$

where module M is determined by the relation

$$M=\left(\frac{\sqrt{a}}{\Delta x}\right)^2\Delta\tau, \tag{9}$$

while the value of M with respect to the stability of the solution must have values less or equal to 0.5.

Explicit scheme for the heat conduction model using derivative of *fractional-order* (2) for homogeneous material has the form (Fig. 2(a))

$$T_{m,p}=MT_{m-1,p-1}-\sum_{j=1}^{N_f}bc_jT_{m,p-j}-2MT_{m,p-1}+MT_{m+1,p-1} \tag{10}$$

and for non-homogeneous material the form

$$T_{m,p}=M_{m-1}T_{m-1,p-1}-\sum_{j=1}^{N_f}bc_jT_{m,p-j}-(M_{m-1}+M_m)T_{m,p-1}+M_mT_{m+1,p-1}. \tag{11}$$

The solution of the fractional derivative of temperature by time based on Grünwald–Letnikov definition

$$\frac{\partial^\alpha T}{\partial\tau^\alpha}=\frac{\sum_{j=0}^{N_f}bc_jT_{m,p-j}}{\Delta\tau^\alpha} \tag{12}$$

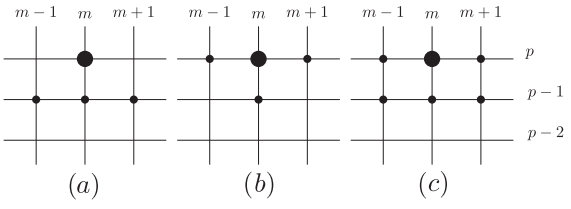

Fig. 1. A stencil for (a) an explicit, (b) an implicit, (c) a Crank–Nicolson scheme for an integer-order derivative.

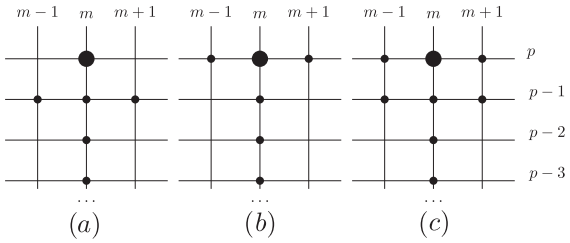

Fig. 2. A stencil for (a) an explicit, (b) an implicit, (c) a Crank–Nicolson scheme for a fractional-order derivative.

by using the principle of "*short memory*", where L is the "length memory" [9], h is the time step and the value of $N(f)$ shall be determined by the following relation

$$N(f) = min\left\{\left[\frac{\tau}{h}\right], \left[\frac{L}{h}\right]\right\}. \tag{13}$$

For the calculation of the binomial coefficients bc_j we can use the relation

$$bc_0 = 1, \quad bc_j = \left(1 - \frac{1+\alpha}{j}\right) \cdot bc_{j-1}, \quad \text{for} \quad j \geqslant 1 \tag{14}$$

and module M_i is determined by the relation

$$M_i = \left(\frac{b_i}{\Delta x}\right)^2 \Delta\tau^{\alpha}. \tag{15}$$

3.2.2. Implicit scheme

In the case of the implicit method usage for the homogeneous material the temperature at a given point m in the new time step p (Fig. 1(b)) and in the case of the boundary condition of the first kind is calculated according to the formula

$$-MT_{m-1,p} + (1+2M)T_{m,p} - MT_{m+1,p} = T_{m,p-1} \tag{16}$$

and for the non-homogeneous body by the formula

$$-M_{m-1}T_{m-1,p} + (1 + M_{m-1} + M_m)T_{m,p} \; - \; M_m T_{m+1,p} = T_{m,p-1}. \tag{17}$$

Fractional shape for the homogeneous material has the form (Fig. 2(b))

$$-MT_{m-1,p} + (1+2M)T_{m,p} - MT_{m+1,p} = -\sum_{j=1}^{N_f} bc_j T_{m,p-j} \tag{18}$$

and for the non-homogeneous body the form

$$-M_{m-1}T_{m-1,p} + (1 + M_{m-1} + M_m)T_{m,p} - M_m T_{m+1,p} = -\sum_{j=1}^{N_f} bc_j T_{m,p-j}. \tag{19}$$

3.2.3. Crank–Nicolson scheme

The Crank–Nicolson scheme is a combination of an explicit and an implicit scheme, i.e. when calculating shall be considered the temperature at that point and neighboring points in the current and previous time step (Fig. 1(c)).

For a homogeneous material it has the form

$$T_{m,p} = \frac{M}{2}\left(T_{m-1,p} - 2T_{m,p} + T_{m+1,p}\right) + \frac{M}{2}\left(T_{m-1,p-1} - 2T_{m,p-1} + T_{m+1,p-1}\right) + T_{m,p-1} \tag{20}$$

and for a non-homogeneous material the form

$$T_{m,p} = \frac{M_m}{2}\left(T_{m-1,p} - 2T_{m,p} + T_{m+1,p}\right) + \frac{M_{m-1}}{2}\left(T_{m-1,p-1} - 2T_{m,p-1} + T_{m+1,p-1}\right) + T_{m,p-1}. \tag{21}$$

The fractional shape for a homogeneous material is given by the following relation (Fig. 2(c))

$$T_{m,p} = \frac{M}{2}\left(T_{m-1,p} - 2T_{m,p} + T_{m+1,p}\right) + \frac{M}{2}\left(T_{m-1,p-1} - 2T_{m,p-1} + T_{m+1,p-1}\right) - \sum_{j=1}^{N_f} bc_j T_{m,p-j} \tag{22}$$

and for a non-homogeneous material

$$T_{m,p} = \frac{1}{2}\left(M_{m-1}T_{m-1,p} - (M_{m-1}+M_m)T_{m,p} + M_m T_{m+1,p}\right) + \frac{1}{2}\left(M_{m-1}T_{m-1,p-1} - (M_{m-1}+M_m)T_{m,p-1} + M_m T_{m+1,p-1}\right) - \sum_{j=1}^{N_f} bc_j T_{m,p-j}. \quad (23)$$

4. Implementation

The implementation was realized in the programming environment MATLAB in which the functions for a model with using integer- (1) and fractional-order (2) derivatives for homogeneous and non-homogeneous material have been created.

4.1. Heat Conduction Toolbox

A library of *m*-functions for the heat conduction model using integer-order derivative called Heat Conduction Toolbox (HCT) is a tool that consists of 7 functions for solving one-dimensional heat conduction with using integer-order derivatives, namely analytical method for a bounded interval and numerical methods (explicit, implicit, Crank–Nicolson scheme) for homogeneous and non-homogeneous material. All implemented functions are published on Mathworks, Inc., Matlab Central File Exchange as Heat Conduction Toolbox [69].

4.2. Fractional Heat Conduction Toolbox

A library of *m*-functions for the heat conduction model using fractional-order derivative called Fractional Heat Conduction Toolbox (FHCT) consists of 7 functions for solving one-dimensional model. Functions include analytical method for a bounded interval and numerical methods for homogeneous and non-homogeneous material. FHCT is published at Mathworks, Inc., Matlab Central File Exchange as Fractional Heat Conduction Toolbox [70].

5. Simulations

Simulations model (1) for homogeneous material can be implemented by using a script `HC_test_h.m` which is a part of the library HCT. The initial conditions, thermophysical properties of the material, spatial division and thickness of the material, time step and the total simulation time, type and values of the boundary condition and the method of solving are defined in the given script. Based on the above definitions the simulation, which is the result of courses temperatures in space and time, can be implemented. As an illustration we give an example of a simulation, where the initial conditions have been defined in the form of the same temperatures of 20 °C after cross-section, as the material was considered brass (λ = 120 W m^{-1} K^{-1}, ρ = 8400 kg m^{-3}, c_p = 380 J kg^{-1} K^{-1}), material thickness (0.03 m), material was divided into six parts in the space, time step (0.1 s), total time simulation (10 s), boundary condition of the 1st kind and temperatures at the edges T_1 = 20 °C and T_2 = 100 °C, and Crank–Nicolson scheme was chosen. Simulation results are shown on Figs. 3 and 4. This is a course of temperatures in time, at which the parameter is the position in space, i.e. 0.015 m (Fig. 3), then it is a course of temperatures in space, wherein the parameter is the time (Fig. 3) and finally it is 3D display temperatures in space and time (Fig. 4).

The part of HCT library is also a script `HC_test_nh.m` which is intended to simulate non-homogeneous material, i.e. material, which is made up of several layers of different materials. The difference between this and the previous script is only in a different enter of the thermophysical properties. Due to the larger number of materials the individual properties are

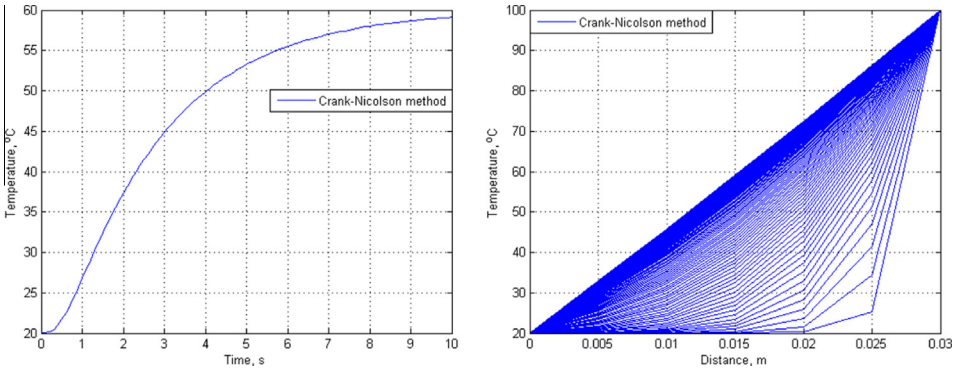

Fig. 3. HCT – the course of temperatures in time and space for homogeneous material.

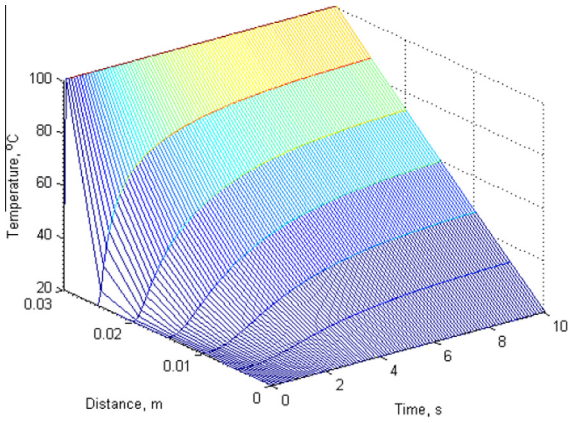

Fig. 4. HCT – 3D display temperatures in time and space for homogeneous material.

given as a vector, i.e. each component of the vector represents a property of a given layer. For example, in the case of the thermal conductivity for six layers and three materials (brass, platinum and silver) of the same thickness it is defined a thermal conductivity vector as follows $\lambda = (120, 120, 7, 7, 428, 428)\,\mathrm{W\,m^{-1}\,K^{-1}}$. It is similar to the density and specific heat capacity. Results of the simulations are shown on figures Figs. 5 and 6.

Another library of the functions, FHCT, is designed for the simulations model (2) where we can set up the derivative of the temperature according to the time from the interval 0 to 2. For the setting, implementing and visualizing of the simulation the script `FHC_test_h.m` is used. This script defines the initial conditions ($T(x,0) = 0$), order of the derivative of the temper-

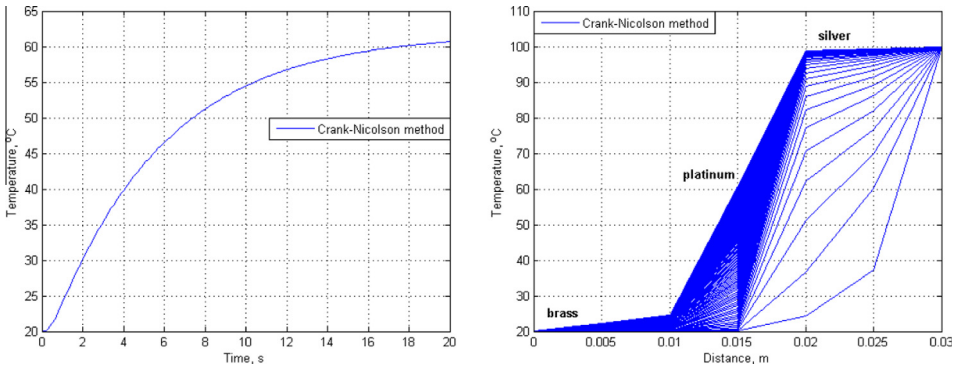

Fig. 5. HCT – the course of temperatures in time and space for non-homogeneous material.

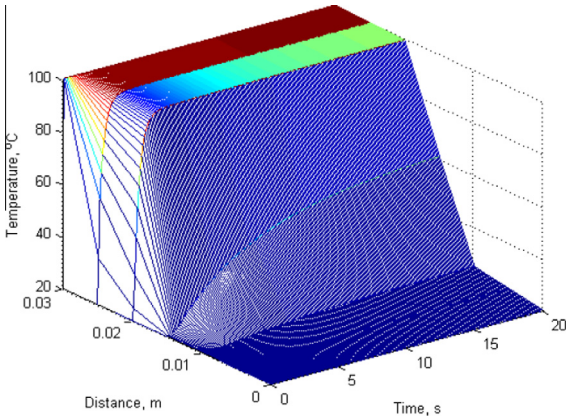

Fig. 6. HCT – 3D display temperatures in time and space for non-homogeneous material.

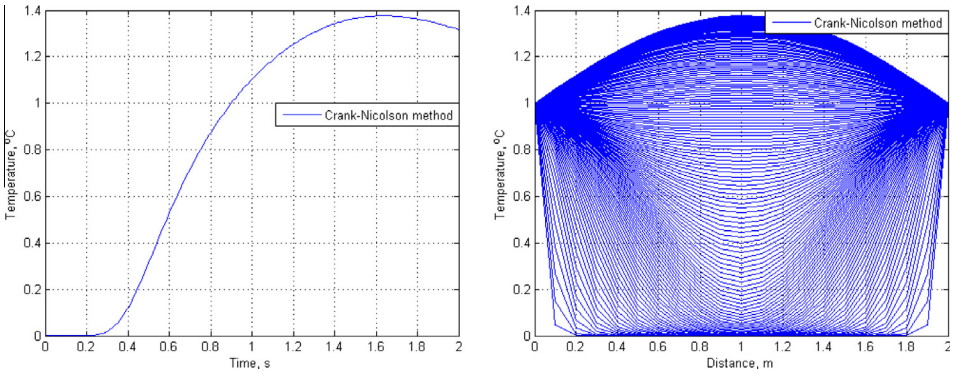

Fig. 7. FHCT – the course of temperatures in time and space for homogeneous material.

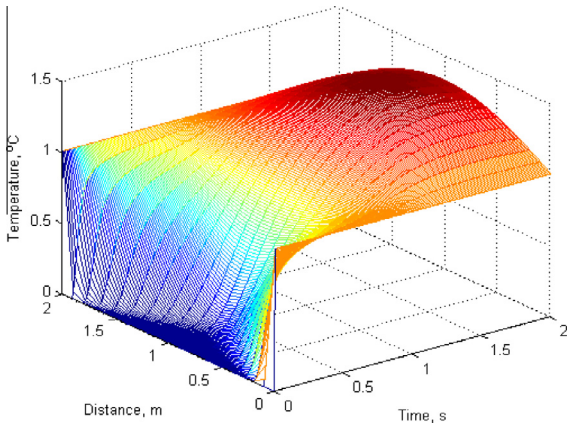

Fig. 8. FHCT – 3D display temperatures in time and space for homogeneous material.

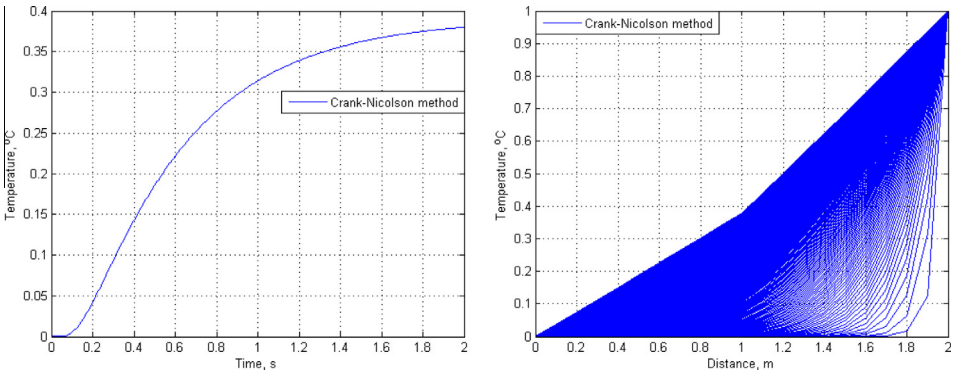

Fig. 9. FHCT – the course of temperatures in time and space for non-homogeneous material.

ature by time (α = 1.5), length memory to calculate the fractional derivative ($N(f) = 200$), material property ($b = 1$ m s$^{-3/4}$), spatial division (20) and material thickness (2 m), time step (0.01 s) and total time simulation (2 s), boundary condition of the 1st kind and values at the edges $T_1 = T_2 = 1$ °C and method of solving (Crank–Nicolson). The results of simulations for the given settings are shown on figures Figs. 7 and 8.

The library FHCT also contains script `FHC_test_nh.m`, which enables to realize the simulations of heat conduction for several layers of different materials. Definition of inputs is the same as for `FHC_test_h.m` with only one difference, i.e. the material property given by a coefficient of b is a vector. Each item of the vector represents a value of the coefficient b of the respective layer. The simulations for the values of the coefficients $b = 1$ for the first half of the thickness and $b = 0.8$ for the second half are given on figures Figs. 9 and 10.

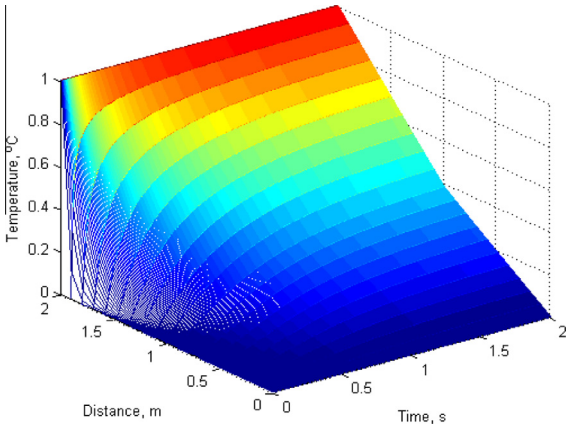

Fig. 10. FHCT – 3D display temperatures in time and space for non-homogeneous material.

6. Conclusion

The models of the heat conduction with using integer and fractional derivatives are listed and described in this article. They have been implemented in MATLAB as two libraries functions, i.e. HCT and FHCT. The possibilities how to use these libraries that beside modeling of the process of the heat conduction allow also to model the processes of the diffusion, wave and so on are illustrated on the examples.

Created more adequate models with using libraries HCT and FHCT have wide using mainly for analysis, design, and control of processes. For these models of processes are characteristic memory systems and ongoing processes, roughness or porosity of the material and also fractality and chaotic behavior of processes and systems.

Libraries are an appropriate tool for the creation of complex models in MATLAB, as evidenced the registered interest of experts in terms of the number of downloaded libraries from the website Matlab Central File Exchange [69,70]. The asset of this work is the use the Grünwald–Letnikov definition for the time derivative in the case of Crank–Nicolson scheme.

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