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*Dedicated to the memory of
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INVESTIGATION OF HEAT DISTRIBUTION USING NON-INTEGER ORDER TIME DERIVATIVE

Summary

This paper presents the analyses of heat distribution based on non-linear order time derivative. The described problem has been demonstrated on a simple rectangular structure made of the silicon. Moreover, the thermal model called Dual-Phase-Lag has been employed to obtain the solution. Furthermore, the new approximation of Dual-Phase-Lag model has been proposed. This modification has been based on Grünwald-Letnikov definition of fractional derivative. The time derivative order, which appears in Fourier-Kirchhoff model, has been modified to non-integer order. Next, received normalized rises of the temperature have been compared with results obtained using Dual-Phase-Lag equation. Then, the orders of the fractional time derivative have been matched to different values of the heat flux and temperature time lags. Eventually, the final formula, which takes into consideration the order of time derivative and both model parameters of Dual-Phase-Lag equation, the heat flux and temperature time lags, is determined. Furthermore, the approximation of the Dual-Phase-Lag heat transfer model is also shown.

Keywords and phrases: Dual-Phase-Lag model, Grünwald Letnikov, heat transfer approximation, Fourier-Kirchhoff modification, non-linear order time derivative

1. Introduction

Currently, the technical and technology development leads to the production of modern electronic devices. One of the characteristic feature of these appliances is their

small size. The restriction related to the small size of the devices demands on electronic producers meaningful reduction of the size of implemented integrated circuits. It causes that significant increase of the generated heat density in electronic appliances is observed. These growths cause that many of thermal problems related to the proper operation of the entire electronic systems occur and lead to the malfunctions and damages. Thus, nowadays one of the crucial aspect regarding the designing of electronic structures is taking into account all new phenomena which occur in such small and modern devices and estimating proper temperature distribution in the structure during its operating process. Due to mentioned reasons, new methodologies of thermal estimation are desired.

1.1. Dual-Phase-Lag model description

The classical thermal approach, which has been used almost through twenty decades, has been established by Fourier [1]. This methodology uses the Fourier's law and Fourier-Kirchhoff equation. The (1) and (2) shows the mathematical description of mentioned physical dependencies.

$$-q(x, y, t) = k\nabla T(x, y, t) \quad (1)$$

$$c_v \frac{\partial T(x, y, t)}{\partial t} = -\nabla \cdot q(x, y, t) + q_{gen}(x, y, t) \quad (2)$$

where $q(x, y, t)$ means the density of the heat flux, while c_v is the volumetric heat capacity, $q_{gen}(x, y, t)$ and $T(x, y, t)$ are the heat generation inside the structure and the temperature function, respectively. In all presented functions, points (x, y) are from two-dimensional space where $x \in \mathbb{R}$, $y \in \mathbb{R}$, and time $t \geq 0$.

Presented approach is suitable for structures made in technology node greater than 180 nm. Received accuracy of thermal simulation is at high level [2]. On the contrary, for structures significantly smaller than mentioned 180 nm, the classical method is not an appropriate choice. First of all, this model does not take into account some physical phenomena, which are especially significant in the case of such small electronic structures. Moreover, it assumes the infinite speed of propagation of the heat and instantaneous heat flux change. These limitations cause meaningful errors during the thermal simulation in the case of nanometric systems [3], [4].

One of the solution, which is getting more and more popular nowadays, is implementation of Dual-Phase-Lag model. This new thermal model was established in 1995 by D. Y. Tzou [5] and contains several modifications of fundamental Fourier-Kirchhoff method. The mathematical formula can be express as follows:

$$\begin{cases} c_v \frac{\partial T(x,y,t)}{\partial t} = -q(x,y,t) \\ q(x,y,t) + \tau_q \frac{\partial q(x,y,t)}{\partial t} = -k \nabla T(x,y,t) - k \tau_T \frac{\partial \nabla T(x,y,t)}{\partial t} \end{cases} \quad (3)$$

where k reflects the value of material thermal conductivity. As it can be seen, this approach contains two new parameters which reflect the heat flux time lag (τ_q) and the temperature time lag (τ_T), respectively. Moreover, if the heat generation is not visible inside the structure and thermal conductivity of investigated materials is independent form temperature, the Dual-Phase-Lag model can be described in the case of second-order formula presented in following equations:

$$\begin{cases} c_v \frac{\partial T(x,y,t)}{\partial t} = -q(x,y,t) \\ c_v \left(\tau_q \frac{\partial^2 T(x,y,t)}{\partial t^2} + \frac{\partial T(x,y,t)}{\partial t} \right) - k \left(\tau_T \frac{\partial \Delta T(x,y,t)}{\partial t} + \Delta T(x,y,t) \right) = 0 \end{cases} \quad (4)$$

One of the biggest advantages of Dual-Phase-Lag model is fact that it can be implemented for both parabolic and hyperbolic cases. Thus, application of this model can be relatively wide.

On the contrary, the direct implementation of Dual-Phase-Lag model can have some difficulties. Firstly, it is characterized by the big computational complexity. In the case when the analyzed structure is characterized by huge number of nodes, the computation of the distribution of the temperature based on full-order model can take definitely much more time. Due to this fact, some approximations of Dual-Phase-Lag model, which allow easier implementation and simulation time reduction, is required. One of that approximation has been shown in [6]. This approach has been based on the model order reduction using Krylov subspaces. In this paper, the other methodology is investigated.

1.2. Grünwald-Letnikov methodology

The analyses carried out in this paper use the fractional derivative based on definition of Grünwald-Letnikov. The form of this mathematical expression can be presented in the following way [7]:

$$D_{0,t}^\alpha u(t) = \sum_{k=0}^{m-1} \frac{u^{(k)}(0)t^{-\alpha+k}}{\Gamma(-\alpha+k+1)} + \frac{1}{m-\alpha} \int_0^t (t-\tau)^{m-\alpha-1} u^{(m)}(\tau) d\tau \quad (5)$$

where $u(t)$ represents the function of t variable for which the determination of derivative should be carried out. The α parameter means the derivatives order. It is worth highlighting that presented mathematical expression is very hard to implement due to numerical issues. Thus, to prepare an easier and more reliable numerical form of

Grünwald-Letnikov derivative, the Finite Difference Method has been applied. Based on this approach, the new formula has been determined and presents as follows [7]:

$$D_{0,t}^{\alpha}u(t)_{GL} = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t^{\alpha}} \sum_{k=0}^N (-1)^k \binom{\alpha}{k} u(t - k\Delta t) \quad (6)$$

where Δt means the difference between the next two points in created mesh, N represents the ceil function of parameter α and $\binom{\alpha}{k}$ is a binomial coefficient.

It was assumed that if the parameter α has a non-integer value, the determination of binomial coefficient uses the gamma functions. Furthermore, to ensure the proper character of the derivative, the formula for N coefficient has been modified and it presents as follows:

$$N = \text{round}(\alpha, 0) \quad (7)$$

where $\text{round}(\alpha, m)$ represents the function which rounds α to m decimal places.

The obtained discrete fractional Grünwald Letnikov derivative formula has the following form:

$$D_{0,t}^{\alpha}u(t)_{GL} = \frac{1}{\Delta t^{\alpha}} \sum_{k=0}^{\text{round}(\alpha, 0)} (-1)^k \frac{\Gamma(\alpha + 1)}{\Gamma(k + 1)\Gamma(\alpha - k + 1)} u(t - k\Delta t) \quad (8)$$

The above expression has been applied to determine the Dual-Phase-Lag approximation scheme, which is the meaningful modification of Fourier-Kirchhoff equation. To employ the Grünwald-Letnikov fractional time derivative in equation (2), the derivative on the left side of this equation has been changed. At the same time, the space derivative observed on the right side of (2) has not been modified. It was assumed that described modification of Fourier-Kirchhoff model is marked by the 'GL FK' abbreviation.

2. Structure

In presented analyses, the two-dimensional rectangular slab has been taken into account. Moreover, it was assumed that structure has been heated in one corner. The heat is generated outside the structure. On the other parts of the slab, the adiabatic or zero boundary conditions have been established. Figure 1 shows the mentioned situation.

As it was previously mentioned to obtain the temperature distribution the numerical method, called Finite Difference Method, has been used. Firstly, the discretization mesh of considered structure has to be determined. It was done according to the following formulas:

$$q_k(t) = q(x, y, t) \quad \text{for} \quad x = i \cdot \Delta x, \quad y = j \cdot \Delta y \quad (9)$$

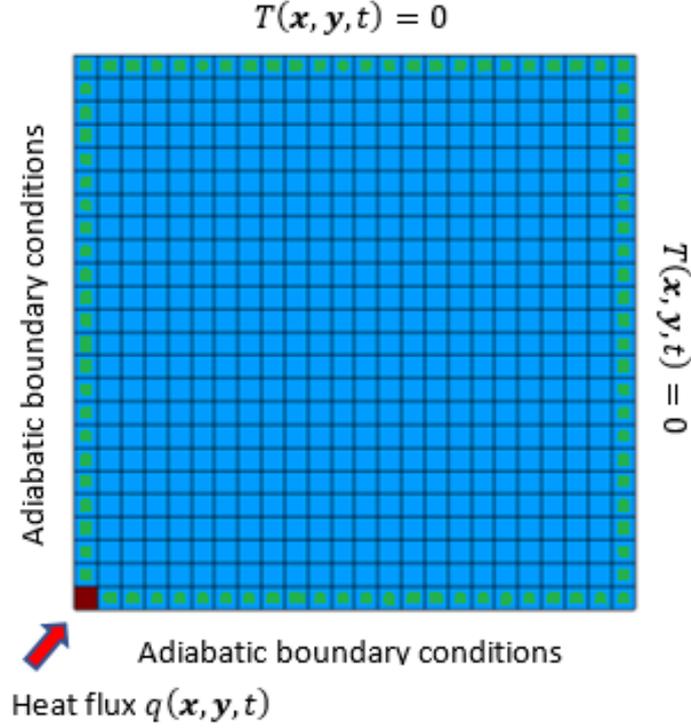


Fig. 1. The visualization of the investigated two-dimensional rectangular slab with marked adiabatic and zero boundary conditions and direction of the heat flux.

$$T_k(t) = T(x, y, t) \quad \text{for} \quad x = i \cdot \Delta x, \quad y = j \cdot \Delta y \quad (10)$$

Moreover, $i \in \{1, 2, \dots, n_l\}, j \in \{1, 2, \dots, n_w\}, k \in \{1, 2, \dots, n_l \cdot n_w\}$. Values n_w and n_l mean the number of mesh nodes along the width and length of the structure, respectively. The expression $n_w \cdot n_l$ reflects to the whole number of nodes. Numbering of nodes starts from the corner, where the heat flux is located, through neighboring nodes on the same side of the structure to the node located on opposite corner. After that, the numbering process is repeated. The procedure of numbering of nodes is finished when the last layer of nodes is numbered. Moreover, the assumption that difference between nodes placed along the width and length of the slab is equal, has been established. The described numbering process of discretization nodes of the square is shown in Figure 2.

The list of initial and boundary conditions which have been used during the temperature distribution is as follows:

$$T_k(t) = 0 \quad \text{for} \quad k \in \{1, 2, \dots, n_l \cdot n_w\}, \quad t = 0 \quad (11)$$

$$q_k(t) = c \quad \text{for} \quad k = 1, \quad t \geq 0, \quad c \in \mathbb{R}_+ \quad (12)$$

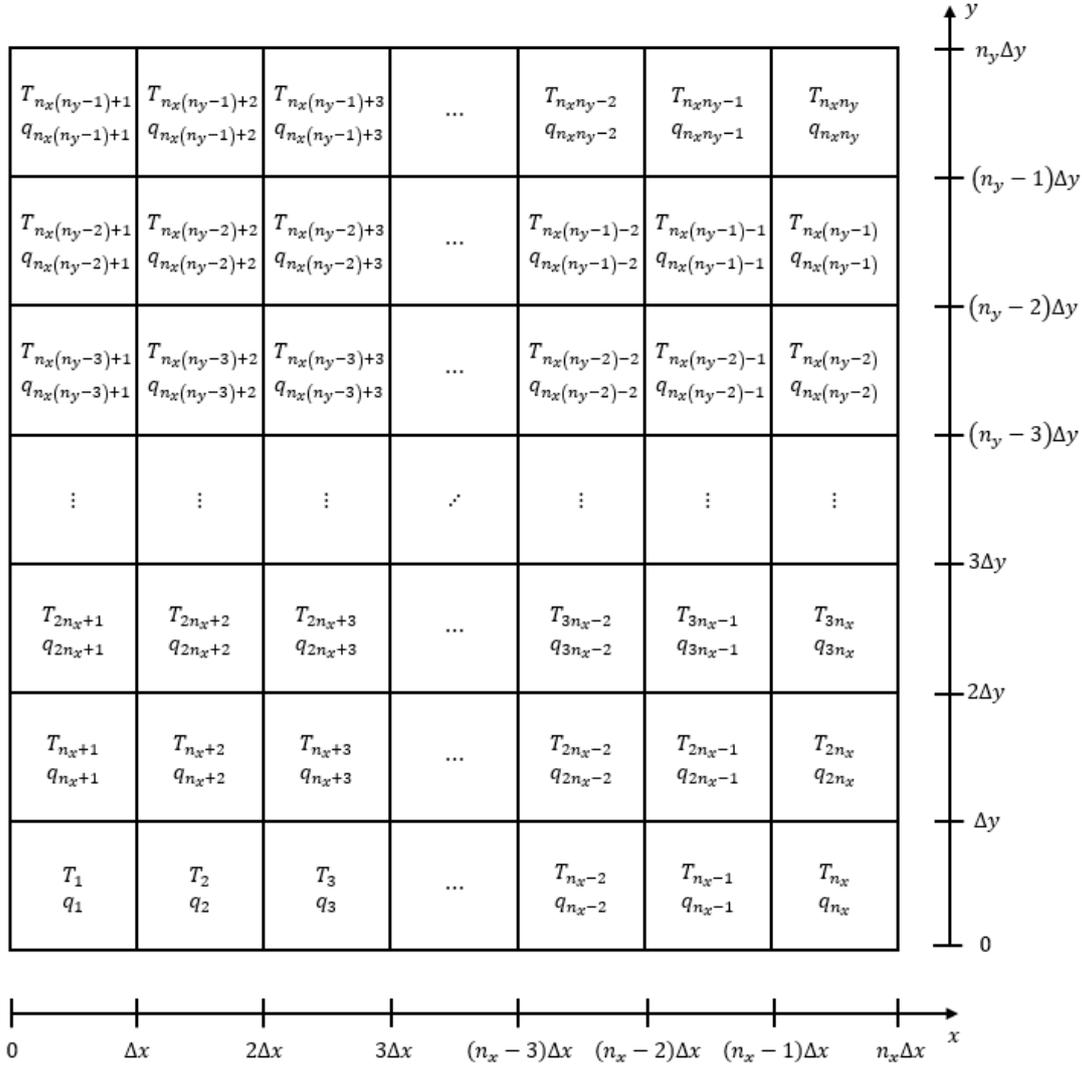


Fig. 2. The graphical representation of the discretization mesh nodes inside the structure and the way of nodes numbering process [6].

$$\begin{aligned}
 T_k(x, y, t) &= 0 \quad \text{for } t \geq 0, \\
 (x = 0 \wedge y > 0) \vee (x = n_l \cdot \Delta x \wedge y \geq 0) \vee \\
 \vee (y = 0 \wedge x > 0) \vee (y = n_w \cdot \Delta y \wedge x \geq 0)
 \end{aligned} \tag{13}$$

3. Simulation and Results

During the simulation process it was assumed that α , order of derivative, comes from the interval $[0.5; 1.5)$. This assumption is caused by the fact that time of derivative is expressed by the first order. Thus, it also implies that in expression (8), the limit value of the superior $\text{round}(\alpha, 0)$ in the sum is equal to unity and the derivative

character is kept.

First analysis is related to the determination of the character of changes of the temperature rises in the node where the heating is observed. During the investigation, the different values of the parameter α has been used and the GL FK model has been applied. The obtained results are presented in Figure 3.

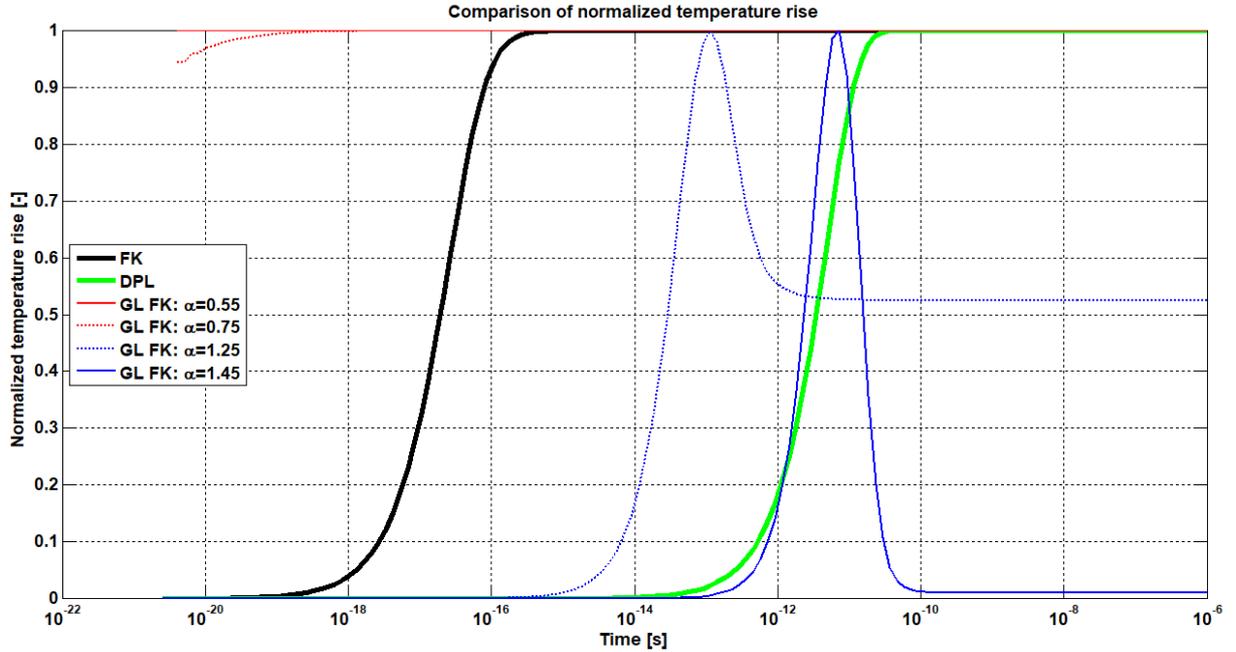


Fig. 3. Comparison of normalized temperature rises in heating node

As it is visible, the received temperature rises for classical FK approach are marked by dark solid line while the DPL results are presented by green solid line. Moreover, the results obtained for GL FK model for different value of order of derivative are demonstrated by solid and dashed red as well as blue lines. Four different values of the α coefficient have been tested.

It occurred that in the case of parameter α smaller than one, the determined curves related to the temperature rises are observed from the left side of the line representing the FK approach. On the contrary, in the case of α greater than 1, the obtained characteristics are visible on the right side of the FK lines. Moreover, in the case of α equal to one, the FK model is observed.

Taking into account previously obtained results, it can be concluded that distributions of the temperature in the case of FK and DPL models have similar characters but temperature rises received by the DPL model are visible later than for FK method. It is caused by the appearance of two time lags in the DPL equation. On the contrary, the dependence of determined temperature rises in the case of GL FK model is different. At the beginning of the simulation time this behavior is similar to the DPL model for chosen time lag parameters, however when the temperature rise

achieves the maximal point, it starts declining. Furthermore, this magnitude of this collapse depends on the time derivative order (α). It is a results of the form of the GL FK formula. Due to this fact, the compensation process has to be applied and its formula is presented below:

$$T_{comp_\alpha}(t) = \max_{s \leq t} \{T_\alpha(x, s)\} \quad (14)$$

In presented formula, the maximal value of the temperature T_α in the period of time $s \leq t$ is chosen.

Next analyses are related to the determination of the temperature distribution in the entire structure. Figure 4 shows the comparison of obtained temperature distribution in both cases, for FK and DPL approaches.

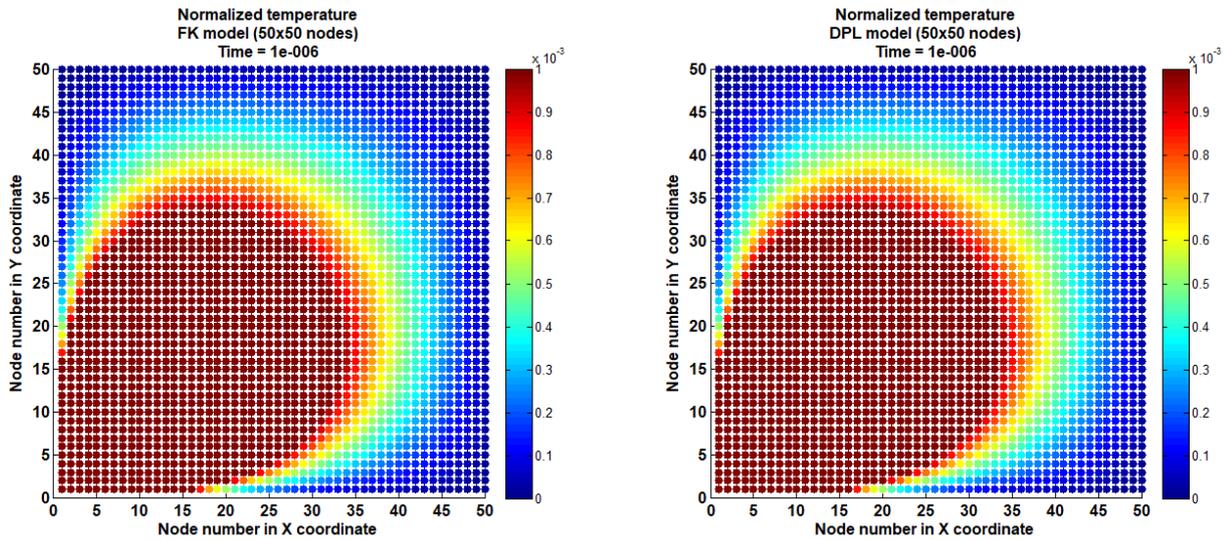


Fig. 4. Comparison of normalized steady state temperatures in the structure in the case of usage of FK and DPL models

As it is visible, the steady state temperature distributions are the same. Moreover, it the temperature distribution for GL FK method in the case of different value of the parameter α have also been compared. Results are presented in Figure 5. In the case of coefficient α smaller than one, the determined temperature distributions are also similar.

However, different behavior is visible in the case of α greater than one. Obtained results are demonstrated in Figure 6.

As it is visible, the significant differences are observed. Obtained temperatures are meaningfully smaller than for α smaller than one. Moreover, the area of the heat propagation is different. Thus, the results do not fit to previously obtained ones. Therefore, the compensation formula 14 has been employed.

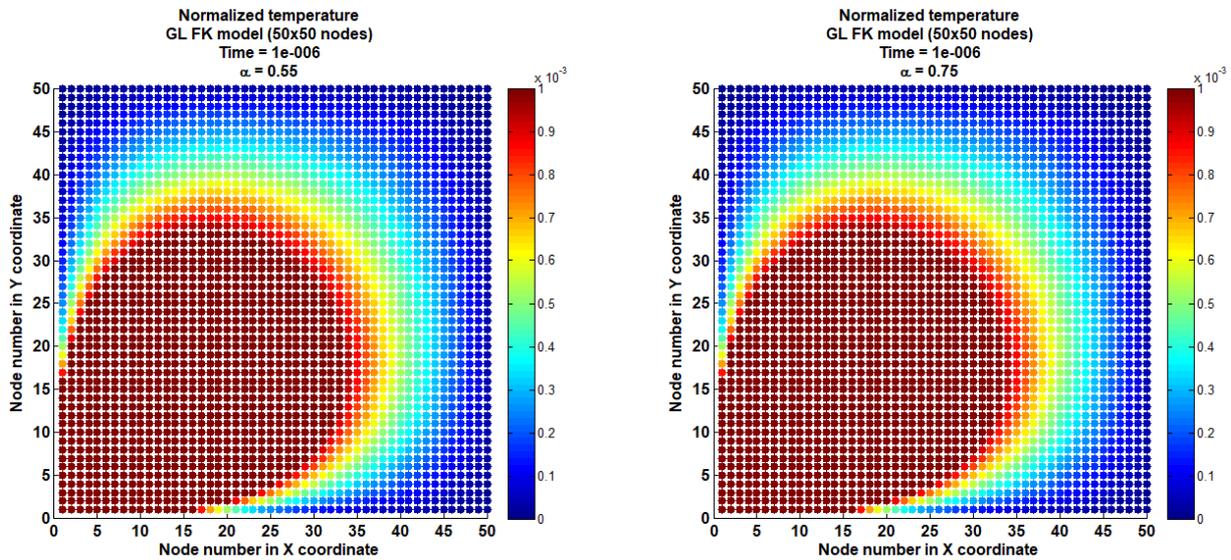


Fig. 5. Comparison of normalized steady state temperatures in the structure in the case of usage of GL FK model for α smaller than 1

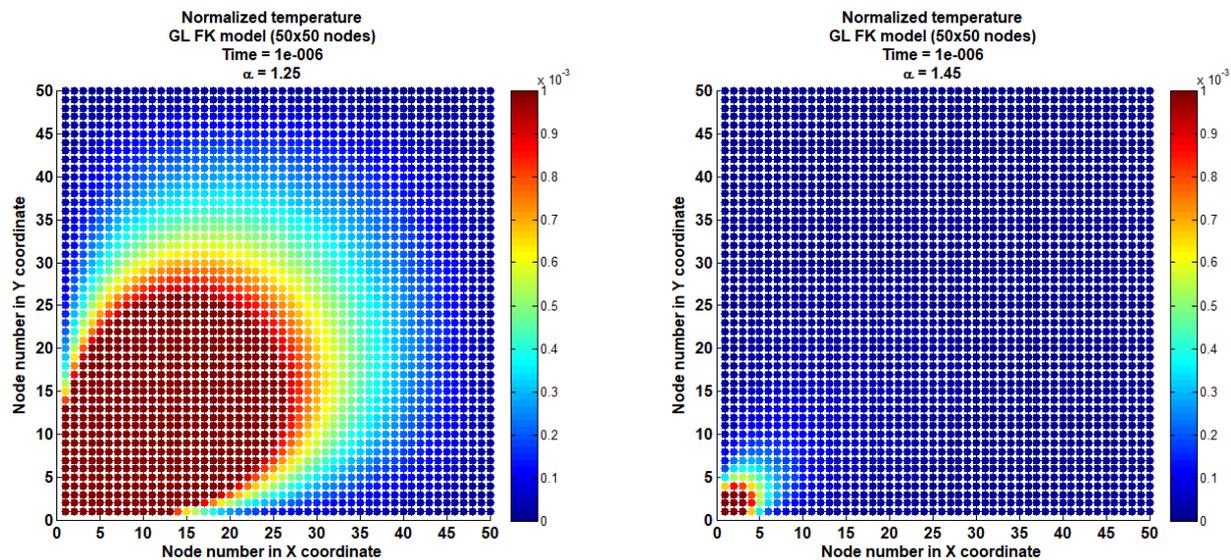


Fig. 6. Comparison of normalized steady state temperatures in the structure in the case of usage of GL FK model for α bigger than 1

After the compensation, the character of curves is similar to these ones obtained using DPL model. Moreover, for certain pair of heat flux and the temperature time lags, the value of the order α has been chosen in a way that the relative error of GL FK curve fitting to the DPL one is as small as possible. Yielded results are shown in Figure 7.

The above figure shows the comparison of normalized temperature rises for chosen parameters of DPL model, marked by black lines, and compensated GL FK model

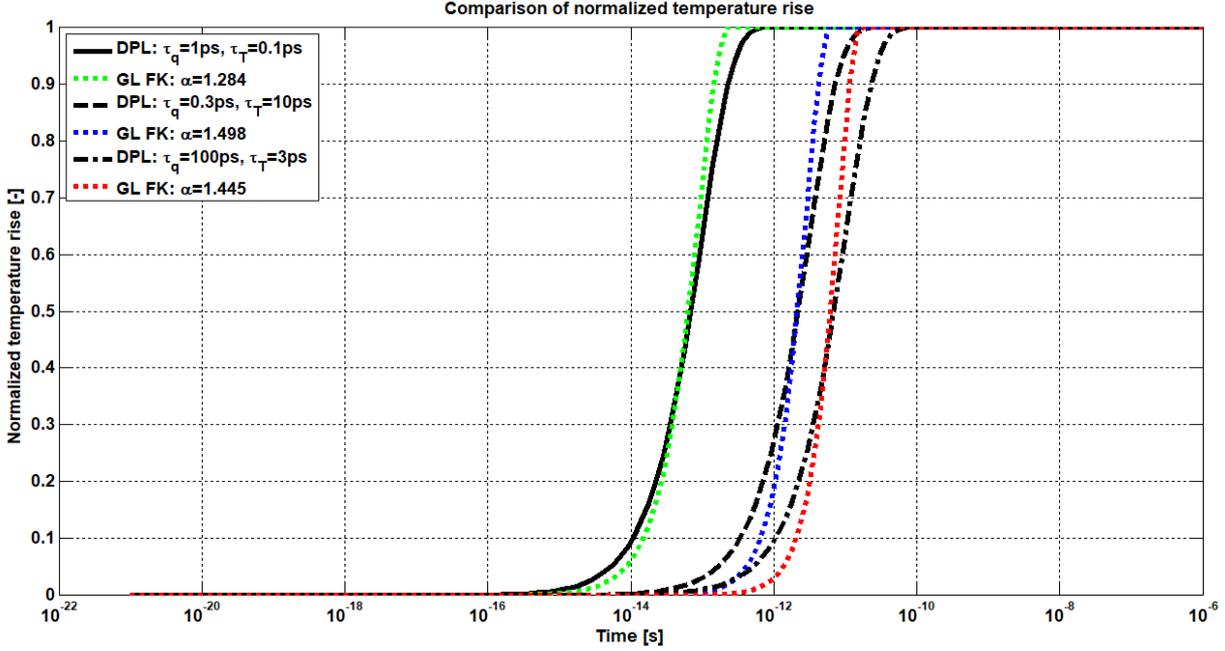


Fig. 7. Comparison of normalized temperature rises in heating for DPL and modified GL FK models

for fitted values of parameter α , marked by the colored lines. As it is visible, three examples of the fitting of compensated GL FK models to the DPL one are presented. It is possible to obtain the similar character of temperature rises for compensated GL FK model which can reflect the DPL model in the heating node. Of course, the range of adequate τ_T, τ_q and α parameters has to be established to obtain quite accurate matching. The dependence between α and time lags can be presented according to the following model:

$$\alpha = a_T \cdot \log_{10} \tau_T + b_T \quad (15)$$

where coefficient a_T and b_T can be described by the below expressions:

$$a_T = a_1 \cdot \tau_q^{b_1} + c_1 \quad (16)$$

$$b_T = a_2 \cdot \tau_q^{b_2} + c_2 \quad (17)$$

Thus, the α is a superposition of logarithmic and power functions. The investigation and determination of the exact values of above parameters have been carried out in [8].

The presented dependence is valid for the heating node. However, in the case of determination of the temperature distribution for the entire structure, obtained results do not coincide. Determined outputs for transient analyses for certain time instants, DPL and GL FK parameters are presented in Figures 8–11.

As it is visible, in every pair of results, the distribution of the temperature in DPL and GL FK is different. Firstly, the temperature rise is similar (Figure 8). However,

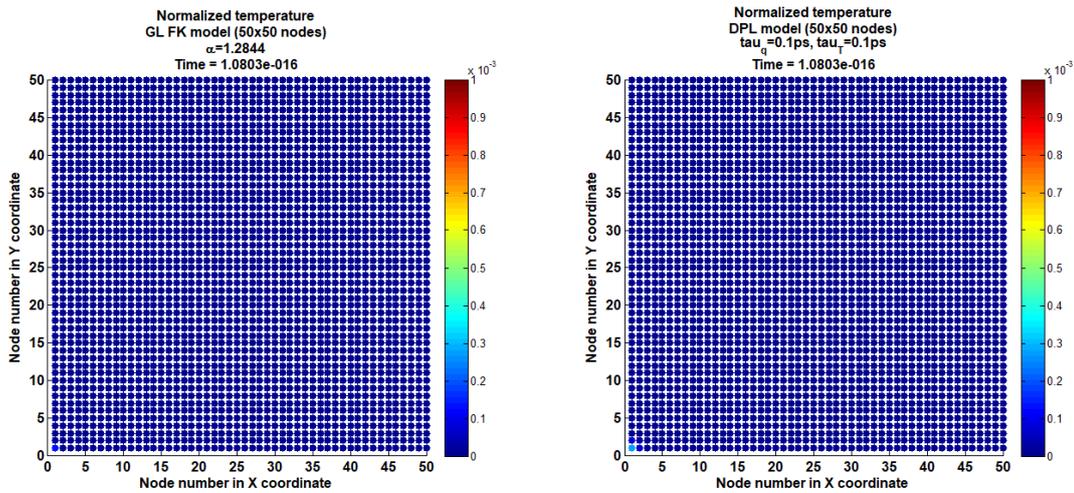


Fig. 8. Comparison of the normalized temperature distribution in the structure in the case of GL FK and DPL models in the initial analysis time

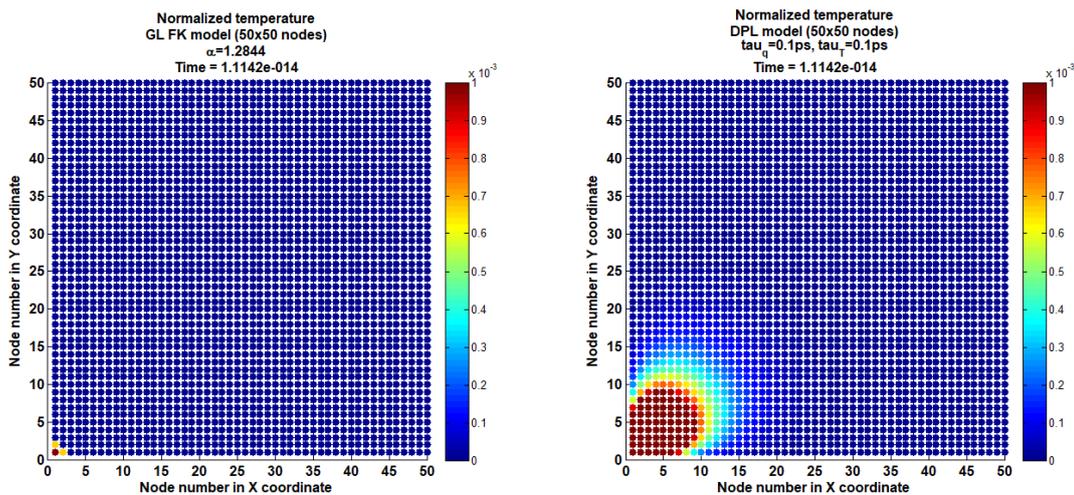


Fig. 9. Comparison of the normalized temperature distribution in the structure in the case of GL FK and DPL models during the initial part of the DPL model temperature rise

after that initial part, the temperature rise is significantly slower for GL FK approach than for DPL one (Figures 9–10). Moreover, at the end of the analysis, the GL FK model generates a little higher temperature than the DPL model. Thus, a bigger part of the structure is characterized by the higher temperatures. This situation is probably caused by the compensation procedure. However, further consideration in this area is needed.

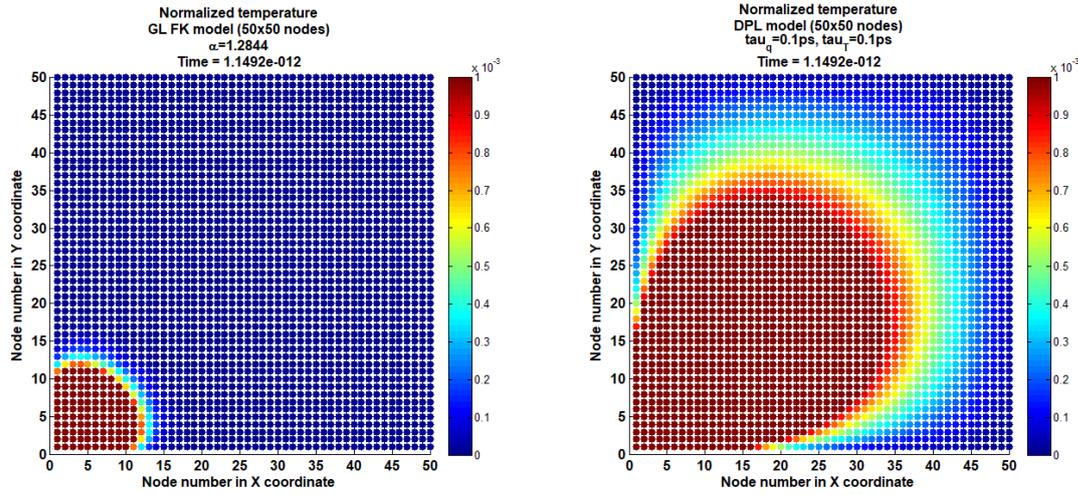


Fig. 10. Comparison of the normalized temperature distribution in the structure in the case of GL FK and DPL models during the final part of the DPL model temperature rise

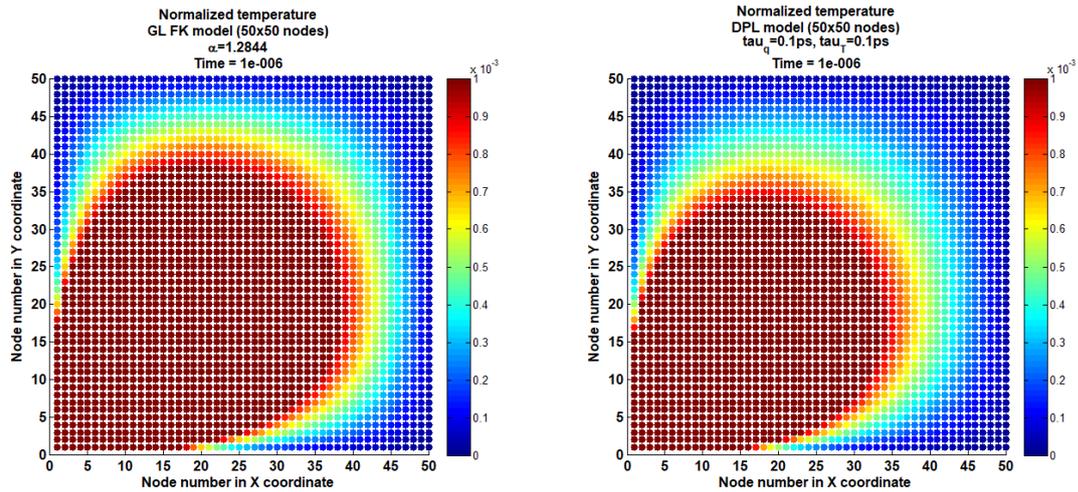


Fig. 11. Comparison of the normalized steady state temperature distribution in the structure in the case of GL FK and DPL models

4. Conclusions

In this paper, the consideration of application of different approaches on non-integer orders to the Dual-Phase-Lag model approximation has been presented. The analyses are based on the comparison of normalized temperature rises obtained using modified Fourier-Kirchhoff model with Grünwald-Letnikov time derivative and the Dual-Phase-Lag one.

Analyses have shown that in some particular cases DPL model can be approximated by the modified FK model, for which the classical time derivative has been replaced by the Grünwald-Letnikov one. However, currently it is limited mainly to

the heating node, for which the relative error is on the acceptable level. Moreover, it is possible only for τ_q , τ_T and α belonging to some limited intervals.

Taking into consideration these limitations, the final formula connecting the time derivative as well as the heat flux and the temperature time lags has been established. The approximation of the DPL model using the modified GL FK one leads to the significant reduction of the time of simulation and reduction of computational power. However, in order to extend the range of applicability this approximation, the further research is needed.

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ANALIZA ROZKŁADU CIEPŁA PRZY UŻYCIU POCHODNEJ TEMPERATURY NIECAŁKOWITEGO RZĘDU W CZASIE

S t r e s z c z e n i e

Artykuł prezentuje analizy dotyczące rozkładu ciepła w nanometrycznych strukturach elektronicznych uzyskane przy użyciu pochodnej temperatury niecałkowitego rzędu w czasie. Opisany problem ukazany został na przykładzie prostej, symetrycznej struktury. W celu wyznaczenia rozkładu ciepła wykorzystano nowoczesny model termiczny o nazwie Dual-Phase-Lag. Ponadto, zaproponowano nowe podejście aproksymujące model Dual-Phase-Lag. Nowy model oparto na klasycznym modelu przepływu ciepła Fouriera-Kirchhoffa, jednakże zamiast klasycznej definicji pochodnej temperatury w czasie, zastosowano definicję pochodnej niecałkowitego rzędu Grünvalda-Letnikova. Następnie, otrzymane znormalizowane przyrosty temperatur przy użyciu tak zmodyfikowanego modelu Fouriera-Kirchhoffa zostały porównane z przyrostami otrzymanymi przy użyciu modelu Dual-Phase-Lag. W dalszej kolejności, rzędy pochodnych temperatury w czasie zostały dopasowane do modeli Dual-Phase-Lag, charakteryzujących się różnymi wartościami opóźnień strumienia ciepła i temperatury. Wyznaczono ponadto ostateczne postaci wzorów przybliżających rząd pochodnych temperatury niecałkowitego rzędu w czasie w zależności od parametrów modelu Dual-Phase-Lag.

Słowa kluczowe: model Dual-Phase-Lag, pochodna Grünvalda-Letnikova, aproksymacja rozkładu ciepła, modyfikacja modelu Fouriera-Kirchhoffa, niecałkowity rząd pochodnej temperatury w czasie